

Thianthrene

Other names:	9,10-Dithiaanthracene Thiaanthrene Thianthren di-o-phenylene disulfide dibenzo-1,4-dithiin
Inchi:	InChI=1S/C12H8S2/c1-2-6-10-9(5-1)13-11-7-3-4-8-12(11)14-10/h1-8H
InchiKey:	GVIJJXMXTUZIOD-UHFFFAOYSA-N
Formula:	C12H8S2
SMILES:	c1ccc2c(c1)Sc1ccccc1S2
Mol. weight [g/mol]:	216.32
CAS:	92-85-3

Physical Properties

Property code	Value	Unit	Source
chs	-7252.50 ± 2.20	kJ/mol	NIST Webbook
chs	-7235.40 ± 0.67	kJ/mol	NIST Webbook
chs	-7250.70 ± 1.60	kJ/mol	NIST Webbook
chs	-7250.30 ± 2.90	kJ/mol	NIST Webbook
chs	-7252.09	kJ/mol	NIST Webbook
chs	-7256.00 ± 4.80	kJ/mol	NIST Webbook
chs	-7253.30 ± 1.40	kJ/mol	NIST Webbook
gf	416.00	kJ/mol	Joback Method
hf	348.93	kJ/mol	Joback Method
hfs	181.30 ± 2.30	kJ/mol	NIST Webbook
hfs	186.60 ± 4.80	kJ/mol	NIST Webbook
hfs	184.20 ± 1.50	kJ/mol	NIST Webbook
hfs	182.60 ± 1.30	kJ/mol	NIST Webbook
hfus	20.62	kJ/mol	Joback Method
hsub	99.40 ± 0.60	kJ/mol	NIST Webbook
hsub	99.39 ± 0.56	kJ/mol	NIST Webbook
hvap	59.86	kJ/mol	Joback Method
ie	7.93	eV	NIST Webbook
ie	7.80 ± 0.03	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-4.55		Crippen Method

logp	4.302		Crippen Method
mcvol	154.260	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	1883.00		NIST Webbook
rinpol	327.90		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	330.13		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1883.00		NIST Webbook
rinpol	327.90		NIST Webbook
rinpol	328.58		NIST Webbook
ss	230.89	J/mol×K	NIST Webbook
tb	639.20	K	NIST Webbook
tc	927.46	K	Joback Method
tf	429.00 ± 1.00	K	NIST Webbook
tf	429.85 ± 0.50	K	NIST Webbook
tt	428.43 ± 0.38	K	NIST Webbook
tt	429.57 ± 0.00	K	NIST Webbook
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.00	J/mol×K	879.57	Joback Method
cpg	406.63	J/mol×K	927.46	Joback Method
cpg	379.09	J/mol×K	783.77	Joback Method
cpg	368.41	J/mol×K	735.87	Joback Method
cpg	356.64	J/mol×K	687.98	Joback Method
cpg	343.58	J/mol×K	640.08	Joback Method
cpg	388.89	J/mol×K	831.67	Joback Method
cps	224.97	J/mol×K	298.15	NIST Webbook
cps	220.17	J/mol×K	298.15	NIST Webbook
hfust	27.55	kJ/mol	429.60	NIST Webbook
hfust	27.55	kJ/mol	429.60	NIST Webbook
hfust	27.56	kJ/mol	429.58	NIST Webbook
hsubt	103.60 ± 0.40	kJ/mol	350.00	NIST Webbook
hsubt	98.60 ± 0.50	kJ/mol	353.00	NIST Webbook
hsubt	97.50 ± 6.30	kJ/mol	353.00	NIST Webbook
hsubt	98.00	kJ/mol	393.00	NIST Webbook

hvapt	69.10	kJ/mol	511.50	NIST Webbook
hvapt	68.70	kJ/mol	511.50	NIST Webbook
hvapt	71.10	kJ/mol	438.00	NIST Webbook
hvapt	61.70	kJ/mol	517.00	NIST Webbook
hvapt	64.50	kJ/mol	517.00	NIST Webbook
hvapt	69.90	kJ/mol	517.00	NIST Webbook
hvapt	72.70	kJ/mol	517.00	NIST Webbook
hvapt	68.40	kJ/mol	499.50	NIST Webbook
hvapt	71.20	kJ/mol	444.50	NIST Webbook
hvapt	67.20	kJ/mol	517.00	NIST Webbook
psub	2.99e-04	kPa	350.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	2.39e-04	kPa	348.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	2.43e-04	kPa	348.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	3.01e-04	kPa	350.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	2.99e-04	kPa	350.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	3.70e-04	kPa	352.11	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	3.68e-04	kPa	352.11	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	3.62e-04	kPa	352.11	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	4.47e-04	kPa	354.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds

psub	4.46e-04	kPa	354.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	4.39e-04	kPa	354.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	5.49e-04	kPa	356.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	5.60e-04	kPa	356.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	5.55e-04	kPa	356.26	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	6.80e-04	kPa	358.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	6.87e-04	kPa	358.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	6.69e-04	kPa	358.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	9.92e-04	kPa	362.05	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	9.95e-04	kPa	362.05	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	9.73e-04	kPa	362.05	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.20e-03	kPa	364.06	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds

psub	1.20e-03	kPa	364.06	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	2.46e-04	kPa	348.10	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.97e-04	kPa	346.12	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.98e-04	kPa	346.12	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	2.00e-04	kPa	346.12	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.61e-04	kPa	344.27	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.63e-04	kPa	344.27	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.61e-04	kPa	344.27	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds
psub	1.17e-03	kPa	364.06	Thermodynamic Study on the Sublimation of Anthracene-Like Compounds

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	477.20	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.86659e+01
Coeff. B	-9.49527e+03
Coeff. C	3.67360e+01
Temperature range (K), min.	460.00
Temperature range (K), max.	674.28

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92853&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Sulfur-Containing Ionic Liquids. Rotating-Bomb Combustion Calorimetry and First Principles	https://www.doi.org/10.1021/je1009366
Sublimation of Anthracene-Like Compounds	https://www.doi.org/10.1021/je100850z
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
2-Ethyl-2-methylimidazolium Thiocyanate:	https://www.chemeo.com/doc/models/crippen_log10ws
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of 9-fluorenone, thianthrene and xanthene in organic solvents: Experimental and computational thermochemical study of two fluorene derivatives:	https://www.doi.org/10.1016/j.fluid.2005.02.016
5-fluoro-2-methylbenzoxazole and 5-fluoro-2-methylbenzothiazole: Redesigning the rotating bomb combustion calorimeter:	https://www.doi.org/10.1016/j.jct.2018.01.022
	http://pubs.acs.org/doi/abs/10.1021/ci990307l
	https://www.doi.org/10.1016/j.jct.2005.08.008

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/17-723-0/Thianthrene.pdf>

Generated by Cheméo on 2025-12-05 13:51:11.842447935 +0000 UTC m=+4690869.372488589.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.