Pentane, 1,1'-thiobis-

Other names:	1,1'-Thiobispentane
	6-THIAUNDECANE
	AMYL SULFIDE
	Di-n-pentyl sulfide
	Diamyl sulfide
	Diamyl sulphide
	Dipentyl sulfide
	Dipentyl sulphide
	Pentyl sulfide
	di-n-Amyl sulfide
	n-Amyl sulfide
Inchi:	InChI=1S/C10H22S/c1-3-5-7-9-11-10-8-6-4-2/h3-10H2,1-2H3
InchiKey:	JOZDADPMWLVEJK-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCCSCCCCC
Mol. weight [g/mol]:	174.35
CAS:	872-10-6

Physical Properties

Property code	Value	Unit	Source
chl	-7429.50	kJ/mol	NIST Webbook
chl	-7415.00 ± 2.00	kJ/mol	NIST Webbook
gf	66.44	kJ/mol	Joback Method
hf	-205.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-267.00 ± 2.00	kJ/mol	NIST Webbook
hfus	25.79	kJ/mol	Joback Method
hvap	62.00 ± 2.00	kJ/mol	NIST Webbook
hvap	62.00	kJ/mol	NIST Webbook
log10ws	-3.89		Crippen Method
logp	4.100		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1276.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1268.00		NIST Webbook

rinpol	1266.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1277.00		NIST Webbook
ripol	1483.00		NIST Webbook
ripol	1461.70		NIST Webbook
ripol	1456.30		NIST Webbook
tb	496.98	K	Joback Method
tc	678.93	K	Joback Method
tf	236.86	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.13	J/mol×K	618.28	Joback Method
cpg	448.38	J/mol×K	648.60	Joback Method
cpg	375.94	J/mol×K	496.98	Joback Method
cpg	391.70	J/mol×K	527.30	Joback Method
cpg	406.81	J/mol×K	557.63	Joback Method
cpg	421.28	J/mol×K	587.95	Joback Method
cpg	461.02	J/mol×K	678.93	Joback Method
hvapt	58.70	kJ/mol	356.00	NIST Webbook
hvapt	57.50	kJ/mol	356.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.20	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62665e+01

Coeff. B	-4.74856e+03
Coeff. C	-8.08560e+01
Temperature range (K), min.	378.03
Temperature range (K), max.	514.31

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.93990e+02
Coeff. B	-4.80618e+04
Coeff. C	-1.31159e+02
Coeff. D	8.65313e-05
Temperature range (K), min.	346.15
Temperature range (K), max.	560.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1846

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1846.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C872106&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume