

Phenanthrene, 9,10-dimethyl-

Other names:	9,10-Dimethylphenanthrene 9,10-Phenanthraquinodimethane
Inchi:	InChI=1S/C16H14/c1-11-12(2)14-8-4-6-10-16(14)15-9-5-3-7-13(11)15/h3-10H,1-2H3
InchiKey:	JUEORGSHIXFSSI-UHFFFAOYSA-N
Formula:	C16H14
SMILES:	<chem>Cc1c(C)c2ccccc2c2ccccc12</chem>
Mol. weight [g/mol]:	206.28
CAS:	604-83-1

Physical Properties

Property code	Value	Unit	Source
chs	-8344.60	kJ/mol	NIST Webbook
gf	380.66	kJ/mol	Joback Method
hf	167.00	kJ/mol	NIST Webbook
hfus	24.11	kJ/mol	Joback Method
hsub	119.50	kJ/mol	NIST Webbook
hvap	58.75	kJ/mol	Joback Method
ie	8.01 ± 0.05	eV	NIST Webbook
log10ws	-6.03		Crippen Method
logp	4.610		Crippen Method
mvol	173.620	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	348.52		NIST Webbook
rinpol	347.90		NIST Webbook
tb	645.06	K	Joback Method
tc	889.67	K	Joback Method
tf	399.46	K	Joback Method
vc	0.667	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.69	J/mol×K	645.06	Joback Method
cpg	445.30	J/mol×K	685.83	Joback Method

cpg	459.74	J/molxK	726.60	Joback Method
cpg	473.15	J/molxK	767.36	Joback Method
cpg	485.63	J/molxK	808.13	Joback Method
cpg	497.31	J/molxK	848.90	Joback Method
cpg	508.31	J/molxK	889.67	Joback Method
dvisc	0.0012344	Paxs	399.46	Joback Method
dvisc	0.0009553	Paxs	440.39	Joback Method
dvisc	0.0007722	Paxs	481.33	Joback Method
dvisc	0.0006454	Paxs	522.26	Joback Method
dvisc	0.0005537	Paxs	563.19	Joback Method
dvisc	0.0004850	Paxs	604.13	Joback Method
dvisc	0.0004320	Paxs	645.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37543e+01
Coeff. B	-4.78678e+03
Coeff. C	-1.19348e+02
Temperature range (K), min.	474.80
Temperature range (K), max.	686.31

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C604831&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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