

Perylene, 1,2,3,3a,4,5,6,7,8,9,9a,10,11,12-tetradecahydro-

Other names:	1,2,3,3a,4,5,6,7,8,9,9a,10,11,12-Tetradecahydroperylene
Inchi:	InChI=1S/C20H26/c1-5-13-6-2-11-17-18-12-4-8-14-7-3-10-16(20(14)18)15(9-1)19(13)17
InchiKey:	JAEIWHRMTMZKDG-UHFFFAOYSA-N
Formula:	C20H26
SMILES:	C1Cc2c3c4c(c5c2C(C1)CCC5)CCCC4CCC3
Mol. weight [g/mol]:	266.42
CAS:	7594-86-7

Physical Properties

Property code	Value	Unit	Source
gf	416.00	kJ/mol	Joback Method
hf	42.61	kJ/mol	Joback Method
hfus	25.85	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.199		Crippen Method
mcvol	225.460	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
tb	753.42	K	Joback Method
tc	1000.36	K	Joback Method
tf	477.38	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.57	J/molxK	753.42	Joback Method
cpg	733.56	J/molxK	794.58	Joback Method
cpg	754.14	J/molxK	835.73	Joback Method
cpg	773.54	J/molxK	876.89	Joback Method
cpg	791.96	J/molxK	918.04	Joback Method
cpg	809.62	J/molxK	959.20	Joback Method
cpg	826.76	J/molxK	1000.36	Joback Method
dvisc	0.0041641	Paxs	477.38	Joback Method

dvisc	0.0035743	Paxs	523.39	Joback Method
dvisc	0.0031447	Paxs	569.39	Joback Method
dvisc	0.0028202	Paxs	615.40	Joback Method
dvisc	0.0025678	Paxs	661.41	Joback Method
dvisc	0.0023666	Paxs	707.41	Joback Method
dvisc	0.0022031	Paxs	753.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7594867&Units=SI
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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