

1,2,3,3a,4,5,5a,6,7,8-Decahydropyrene

Inchi:	InChI=1S/C16H20/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h7,9,12,14H,1-6
InchiKey:	MNXFZXVRYXNOBW-UHFFFAOYSA-N
Formula:	C16H20
SMILES:	c1cc2c3c4c1CCCC4CCC3CCC2
Mol. weight [g/mol]:	212.33
CAS:	14698-02-3

Physical Properties

Property code	Value	Unit	Source
gf	345.22	kJ/mol	Joback Method
hf	61.13	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	55.69	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.320		Crippen Method
mcvol	179.960	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
tb	636.26	K	Joback Method
tc	878.71	K	Joback Method
tf	388.60	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.87	J/molxK	636.26	Joback Method
cpg	525.86	J/molxK	676.67	Joback Method
cpg	545.29	J/molxK	717.08	Joback Method
cpg	563.31	J/molxK	757.48	Joback Method
cpg	580.10	J/molxK	797.89	Joback Method
cpg	595.82	J/molxK	838.30	Joback Method
cpg	610.65	J/molxK	878.71	Joback Method
dvisc	0.0027078	Paxs	388.60	Joback Method
dvisc	0.0023288	Paxs	429.88	Joback Method

dvisc	0.0020565	Paxs	471.15	Joback Method
dvisc	0.0018528	Paxs	512.43	Joback Method
dvisc	0.0016954	Paxs	553.71	Joback Method
dvisc	0.0015706	Paxs	594.98	Joback Method
dvisc	0.0014695	Paxs	636.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14698023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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