

Tetrahydroaplotaxene

Inchi:	InChI=1S/C17H32/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3,15,17H,1,4-14,16H2,2
InchiKey:	ZCNSOBXQEHNQMJ-ICFOKQHNSA-N
Formula:	C17H32
SMILES:	C=CCCCCCC=CCCCCCCC
Mol. weight [g/mol]:	236.44

Physical Properties

Property code	Value	Unit	Source
gf	260.32	kJ/mol	Joback Method
hf	-151.56	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	52.72	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	6.430		Crippen Method
mvol	241.790	ml/mol	McGowan Method
pc	1316.56	kPa	Joback Method
ripol	1758.00		NIST Webbook
ripol	1758.00		NIST Webbook
tb	589.20	K	Joback Method
tc	755.29	K	Joback Method
tf	274.51	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.58	J/molxK	589.20	Joback Method
cpg	645.48	J/molxK	616.88	Joback Method
cpg	663.56	J/molxK	644.56	Joback Method
cpg	680.85	J/molxK	672.25	Joback Method
cpg	697.39	J/molxK	699.93	Joback Method
cpg	713.21	J/molxK	727.61	Joback Method
cpg	728.34	J/molxK	755.29	Joback Method
dvisc	0.0042107	Paxs	274.51	Joback Method

dvisc	0.0014518	Paxs	326.96	Joback Method
dvisc	0.0006719	Paxs	379.41	Joback Method
dvisc	0.0003749	Paxs	431.86	Joback Method
dvisc	0.0002374	Paxs	484.30	Joback Method
dvisc	0.0001644	Paxs	536.75	Joback Method
dvisc	0.0001215	Paxs	589.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R337185&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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