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=CCCCCCCCC
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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0014518	Pa×s	326.96	Joback Method
dvisc	0.0006719	Pa×s	379.41	Joback Method
dvisc	0.0003749	Pa×s	431.86	Joback Method
dvisc	0.0002374	Pa×s	484.30	Joback Method
dvisc	0.0001644	Pa×s	536.75	Joback Method
dvisc	0.0001215	Pa×s	589.20	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=R337185&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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