(Z,Z)-1,8,11-Heptadecatriene

Other names: Dihydroaplotaxene
(Z,Z)-heptadeca-1,8,11-triene
Inchi: InChI=1S/C17H30/c1-3-5-7-9-11-13-15-17-16-14-12-10-8-6-4-2/h3,12,14-15,17H,1,4-11,
InchiKey: XFZBIINLEPBMDY-NERFDCTISA-N
Formula: C17H30
SMILES: C=CCCCCCC=CCC=CCCCCC
Mol. weight [g/mol]: 234.42
CAS: 56134-03-3

Physical Properties

Property code	Value	Unit	Source
gf	340.54	kJ/mol	Joback Method
hf	-34.34	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	52.68	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.206		Crippen Method
mcvol	237.490	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	1664.60		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1655.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1787.00		NIST Webbook
tb	593.36	K	Joback Method
tc	765.28	K	Joback Method
tf	269.43	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	607.56	J/mol×K	593.36	Joback Method
cpg	626.14	J/mol×K	622.01	Joback Method
cpg	643.85	J/mol×K	650.67	Joback Method
cpg	660.74	J/mol×K	679.32	Joback Method
cpg	676.86	J/mol×K	707.97	Joback Method
cpg	692.24	J/mol×K	736.62	Joback Method
cpg	706.93	J/mol×K	765.28	Joback Method
dvisc	0.0039750	Pa×s	269.43	Joback Method
dvisc	0.0013044	Pa×s	323.42	Joback Method
dvisc	0.0005888	Pa×s	377.41	Joback Method
dvisc	0.0003243	Pa×s	431.39	Joback Method
dvisc	0.0002040	Pa×s	485.38	Joback Method
dvisc	0.0001408	Pa×s	539.37	Joback Method
dvisc	0.0001039	Pa×s	593.36	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56134033&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume