

(7R,8S)-cis-7,8-epoxy-octadecane [(+)-monachalure]

Inchi: InChI=1S/C18H36O/c1-3-5-7-9-10-11-12-14-16-18-17(19-18)15-13-8-6-4-2/h17-18H,3-16H
InchiKey: ABMJUFOPOPEJRG-ROUUACIJSA-N
Formula: C18H36O
SMILES: CCCCCCCCCC1OC1CCCCC
Mol. weight [g/mol]: 268.48

Physical Properties

Property code	Value	Unit	Source
gf	67.60	kJ/mol	Joback Method
hf	-494.39	kJ/mol	Joback Method
hfus	49.56	kJ/mol	Joback Method
hvap	59.78	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	6.255		Crippen Method
mcvol	259.490	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	1971.00		NIST Webbook
rinpol	1971.00		NIST Webbook
tb	640.26	K	Joback Method
tc	807.77	K	Joback Method
tf	332.89	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.72	J/mol×K	640.26	Joback Method
cpg	771.06	J/mol×K	668.18	Joback Method
cpg	790.51	J/mol×K	696.10	Joback Method
cpg	809.09	J/mol×K	724.02	Joback Method
cpg	826.85	J/mol×K	751.93	Joback Method
cpg	843.82	J/mol×K	779.85	Joback Method
cpg	860.03	J/mol×K	807.77	Joback Method
dvisc	0.0028162	Pa×s	332.89	Joback Method

dvisc	0.0015636	Pa×s	384.12	Joback Method
dvisc	0.0009971	Pa×s	435.35	Joback Method
dvisc	0.0006990	Pa×s	486.57	Joback Method
dvisc	0.0005243	Pa×s	537.80	Joback Method
dvisc	0.0004135	Pa×s	589.03	Joback Method
dvisc	0.0003387	Pa×s	640.26	Joback Method

Sources

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=R501623&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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