(6Z,9Z)-Trans-11,12-Epoxyhenicosa-6,9-diene

Other names: (6Z,9Z,11S,12S)-trans-11,12-epoxyhenicosa-6,9-diene
Inchi: InChI=1S/C21H38O/c1-3-5-7-9-11-13-15-17-19-21-20(22-21)18-16-14-12-10-8-6-4-2/h11
InchiKey: AZNAATMZDDJQSS-OHNCOSGTSA-N
Formula: C21H38O
SMILES: CCCCCC=CCC=CC1OC1CCCCCCCCC
Mol. weight [g/mol]: 306.53

Physical Properties

Property code	Value	Unit	Source
gf	253.30	kJ/mol	Joback Method
hf	-321.87	kJ/mol	Joback Method
hfus	57.74	kJ/mol	Joback Method
hvap	66.37	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.977		Crippen Method
mcvol	293.160	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	2200.00		NIST Webbook
ripol	2548.00		NIST Webbook
tb	717.22	K	Joback Method
tc	894.59	K	Joback Method
tf	356.54	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.63	J/mol×K	717.22	Joback Method
cpg	905.11	J/mol×K	746.78	Joback Method
cpg	924.63	J/mol×K	776.34	Joback Method
cpg	943.25	J/mol×K	805.91	Joback Method
cpg	961.03	J/mol×K	835.47	Joback Method
cpg	978.04	J/mol×K	865.03	Joback Method
cpg	994.32	J/mol×K	894.59	Joback Method

dvisc	0.0021496	Pa×s	356.54	Joback Method
dvisc	0.0010789	Pa×s	416.65	Joback Method
dvisc	0.0006443	Pa×s	476.77	Joback Method
dvisc	0.0004318	Pa×s	536.88	Joback Method
dvisc	0.0003137	Pa×s	596.99	Joback Method
dvisc	0.0002416	Pa×s	657.11	Joback Method
dvisc	0.0001944	Pa×s	717.22	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=U360452&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
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

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