2-(4-Methyl-pentyl)-3-decyl-oxirane

Other names: 2-(5-Methyl-pentyl)-3-decyl-oxirane
Inchi: InChI=1S/C18H36O/c1-4-5-6-7-8-9-10-11-14-17-18(19-17)15-12-13-16(2)3/h16-18H,4-15
InchiKey: MYAXSLNSJQGASK-UHFFFAOYSA-N
Formula: C18H36O
SMILES: CCCCCCCCCCC1OC1CCCC(C)C
Mol. weight [g/mol]: 268.48

Physical Properties

Property code	Value	Unit	Source
gf	65.16	kJ/mol	Joback Method
hf	-499.67	kJ/mol	Joback Method
hfus	46.04	kJ/mol	Joback Method
hvap	59.39	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	6.111		Crippen Method
mcvol	259.490	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	1896.00		NIST Webbook
tb	639.82	K	Joback Method
tc	809.59	K	Joback Method
tf	317.89	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.06	J/mol×K	639.82	Joback Method
cpg	845.42	J/mol×K	781.29	Joback Method
cpg	828.26	J/mol×K	753.00	Joback Method
cpg	810.28	J/mol×K	724.70	Joback Method
cpg	791.44	J/mol×K	696.41	Joback Method
cpg	771.71	J/mol×K	668.11	Joback Method
cpg	861.80	J/mol×K	809.59	Joback Method
dvisc	0.0003148	Pa×s	639.82	Joback Method

dvisc	0.0003905	Pa×s	586.16	Joback Method
dvisc	0.0005059	Pa×s	532.51	Joback Method
dvisc	0.0006946	Pa×s	478.85	Joback Method
dvisc	0.0010331	Pa×s	425.20	Joback Method
dvisc	0.0017232	Pa×s	371.54	Joback Method
dvisc	0.0034163	Pa×s	317.89	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=R489464&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume