

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,4-1
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.06	J/molxK	639.82	Joback Method
cpg	771.71	J/molxK	668.11	Joback Method
cpg	791.44	J/molxK	696.41	Joback Method
cpg	810.28	J/molxK	724.70	Joback Method
cpg	828.26	J/molxK	753.00	Joback Method
cpg	845.42	J/molxK	781.29	Joback Method
cpg	861.80	J/molxK	809.59	Joback Method
dvisc	0.0034163	Paxs	317.89	Joback Method

dvisc	0.0017232	Paxs	371.54	Joback Method
dvisc	0.0010331	Paxs	425.20	Joback Method
dvisc	0.0006946	Paxs	478.85	Joback Method
dvisc	0.0005059	Paxs	532.51	Joback Method
dvisc	0.0003905	Paxs	586.16	Joback Method
dvisc	0.0003148	Paxs	639.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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