

2-(5-Methyl-heptyl)-3-nonyl-oxirane

Inchi:	InChI=1S/C19H38O/c1-4-6-7-8-9-10-11-15-18-19(20-18)16-13-12-14-17(3)5-2/h17-19H,4
InchiKey:	ONWFPAUPIWYIBF-UHFFFAOYSA-N
Formula:	C19H38O
SMILES:	CCCCCCCCC1OC1CCCC(C)CC
Mol. weight [g/mol]:	282.50

Physical Properties

Property code	Value	Unit	Source
gf	73.58	kJ/mol	Joback Method
hf	-520.31	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.501		Crippen Method
mcvol	273.580	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	662.70	K	Joback Method
tc	832.43	K	Joback Method
tf	329.16	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.45	J/molxK	662.70	Joback Method
cpg	830.42	J/molxK	690.99	Joback Method
cpg	850.44	J/molxK	719.28	Joback Method
cpg	869.55	J/molxK	747.57	Joback Method
cpg	887.80	J/molxK	775.86	Joback Method
cpg	905.21	J/molxK	804.15	Joback Method
cpg	921.83	J/molxK	832.43	Joback Method
dvisc	0.0033344	Paxs	329.16	Joback Method

dvisc	0.0016515	Paxs	384.75	Joback Method
dvisc	0.0009768	Paxs	440.34	Joback Method
dvisc	0.0006499	Paxs	495.93	Joback Method
dvisc	0.0004694	Paxs	551.52	Joback Method
dvisc	0.0003599	Paxs	607.11	Joback Method
dvisc	0.0002885	Paxs	662.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R489444&Units=SI
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

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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