

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

ONWFPAUPIWYIBF-UHFFFAOYSA-N

C19H38O

CCCCCCCCC1OC1CCCC(C)CC

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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0016515	Pa×s	384.75	Joback Method
dvisc	0.0009768	Pa×s	440.34	Joback Method
dvisc	0.0006499	Pa×s	495.93	Joback Method
dvisc	0.0004694	Pa×s	551.52	Joback Method
dvisc	0.0003599	Pa×s	607.11	Joback Method
dvisc	0.0002885	Pa×s	662.70	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=R489444&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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