

Oxiraneundecanoic acid, 3-pentyl-, methyl ester, cis-

Other names:	Methyl 11-(3-pentyl-2-oxiranyl)undecanoate, cis-
Inchi:	InChI=1S/C19H36O3/c1-3-4-11-14-17-18(22-17)15-12-9-7-5-6-8-10-13-16-19(20)21-2/h1
InchiKey:	CJIHQKTUUVMSU-UHFFFAOYSA-N
Formula:	C19H36O3
SMILES:	CCCCC1OC1CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	312.49
CAS:	38520-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-157.90	kJ/mol	Joback Method
hf	-759.83	kJ/mol	Joback Method
hfus	54.94	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.408		Crippen Method
mcvol	281.020	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2437.00		NIST Webbook
tb	739.43	K	Joback Method
tc	916.65	K	Joback Method
tf	416.32	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.93	J/molxK	739.43	Joback Method
cpg	960.59	J/molxK	887.11	Joback Method
cpg	945.00	J/molxK	857.58	Joback Method
cpg	928.58	J/molxK	828.04	Joback Method
cpg	911.28	J/molxK	798.50	Joback Method
cpg	893.07	J/molxK	768.97	Joback Method
cpg	975.36	J/molxK	916.65	Joback Method

dvisc	0.0002595	Paxs	739.43	Joback Method
dvisc	0.0003186	Paxs	685.58	Joback Method
dvisc	0.0004050	Paxs	631.73	Joback Method
dvisc	0.0005385	Paxs	577.88	Joback Method
dvisc	0.0007592	Paxs	524.02	Joback Method
dvisc	0.0011578	Paxs	470.17	Joback Method
dvisc	0.0019696	Paxs	416.32	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=C38520308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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