

3-Hexyl-oxirane-2-carboxylic acid methyl ester

Inchi:	InChI=1S/C10H18O3/c1-3-4-5-6-7-8-9(13-8)10(11)12-2/h8-9H,3-7H2,1-2H3
InchiKey:	CYFDJMXHODROJG-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCCCCCC1OC1C(=O)OC
Mol. weight [g/mol]:	186.25

Physical Properties

Property code	Value	Unit	Source
gf	-233.68	kJ/mol	Joback Method
hf	-574.07	kJ/mol	Joback Method
hfus	31.63	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.897		Crippen Method
mvol	154.210	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	533.51	K	Joback Method
tc	717.59	K	Joback Method
tf	314.89	K	Joback Method
vc	0.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.72	J/molxK	533.51	Joback Method
cpg	401.63	J/molxK	564.19	Joback Method
cpg	415.86	J/molxK	594.87	Joback Method
cpg	429.42	J/molxK	625.55	Joback Method
cpg	442.34	J/molxK	656.23	Joback Method
cpg	454.64	J/molxK	686.91	Joback Method
cpg	466.33	J/molxK	717.59	Joback Method
dvisc	0.0021260	Paxs	314.89	Joback Method

dvisc	0.0014878	Paxs	351.33	Joback Method
dvisc	0.0011135	Paxs	387.76	Joback Method
dvisc	0.0008759	Paxs	424.20	Joback Method
dvisc	0.0007156	Paxs	460.64	Joback Method
dvisc	0.0006023	Paxs	497.07	Joback Method
dvisc	0.0005189	Paxs	533.51	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=R249271&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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