2-Heptyl-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C11H20O3/c1-3-4-5-6-7-8-11(9-14-11)10(12)13-2/h3-9H2,1-2H3
InchiKey: UTZQYBPIBOKLLR-UHFFFAOYSA-N
Formula: C11H20O3
SMILES: CCCCCCCC1(C(=O)OC)CO1
Mol. weight [g/mol]: 200.27

Physical Properties

Property code	Value	Unit	Source
gf	-223.04	kJ/mol	Joback Method
hf	-559.13	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	52.51	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.289		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	561.30	K	Joback Method
tc	750.29	K	Joback Method
tf	354.30	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.85	J/mol×K	561.30	Joback Method
cpg	447.82	J/mol×K	592.80	Joback Method
cpg	462.02	J/mol×K	624.30	Joback Method
cpg	475.51	J/mol×K	655.80	Joback Method
cpg	488.39	J/mol×K	687.29	Joback Method
cpg	500.74	J/mol×K	718.79	Joback Method
cpg	512.64	J/mol×K	750.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
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