3-(3-Carboxy-propyl)-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C8H12O5/c1-12-8(11)7-5(13-7)3-2-4-6(9)10/h5,7H,2-4H2,1H3,(H,9,10)
InchiKey: FSHLQCGOAFXLCO-UHFFFAOYSA-N
Formula: C8H12O5
SMILES: COC(=O)C1OC1CCCC(=O)O
Mol. weight [g/mol]: 188.18

Physical Properties

Property code	Value	Unit	Source
gf	-516.26	kJ/mol	Joback Method
hf	-797.60	kJ/mol	Joback Method
hfus	32.13	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	0.182		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1390.00		NIST Webbook
tb	633.80	K	Joback Method
tc	820.50	K	Joback Method
tf	403.10	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.93	J/mol×K	633.80	Joback Method
cpg	374.15	J/mol×K	664.92	Joback Method
cpg	383.83	J/mol×K	696.03	Joback Method
cpg	392.99	J/mol×K	727.15	Joback Method
cpg	401.64	J/mol×K	758.27	Joback Method
cpg	409.79	J/mol×K	789.39	Joback Method
cpg	417.47	J/mol×K	820.50	Joback Method
dvisc	0.0030986	Pa×s	403.10	Joback Method
dvisc	0.0016701	Pa×s	441.55	Joback Method

dvisc	0.0009938	Pa×s	480.00	Joback Method
dvisc	0.0006387	Pa×s	518.45	Joback Method
dvisc	0.0004364	Pa×s	556.90	Joback Method
dvisc	0.0003132	Pa×s	595.35	Joback Method
dvisc	0.0002340	Pa×s	633.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249251&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
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