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

Inchi: InChI=1S/C7H10O5/c1-11-7(10)6-4(12-6)2-3-5(8)9/h4,6H,2-3H2,1H3,(H,8,9)
InchiKey: TZJFDVISKBEVHZ-UHFFFAOYSA-N
Formula: C7H10O5
SMILES: COC(=O)C1OC1CCC(=O)O
Mol. weight [g/mol]: 174.15

Physical Properties

Property code	Value	Unit	Source
gf	-524.68	kJ/mol	Joback Method
hf	-776.96	kJ/mol	Joback Method
hfus	29.54	kJ/mol	Joback Method
hvap	67.87	kJ/mol	Joback Method
log10ws	0.08		Crippen Method
logp	-0.208		Crippen Method
mcvol	119.380	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
rinpol	1292.00		NIST Webbook
tb	610.92	K	Joback Method
tc	799.49	K	Joback Method
tf	391.83	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.53	J/mol×K	610.92	Joback Method
cpg	358.90	J/mol×K	768.06	Joback Method
cpg	351.37	J/mol×K	736.63	Joback Method
cpg	343.38	J/mol×K	705.21	Joback Method
cpg	334.92	J/mol×K	673.78	Joback Method
cpg	325.97	J/mol×K	642.35	Joback Method
cpg	365.99	J/mol×K	799.49	Joback Method
dvisc	0.0002682	Pa×s	610.92	Joback Method
dvisc	0.0003576	Pa×s	574.40	Joback Method

dvisc	0.0004960	Pa×s	537.89	Joback Method
dvisc	0.0007214	Pa×s	501.38	Joback Method
dvisc	0.0011129	Pa×s	464.86	Joback Method
dvisc	0.0018484	Pa×s	428.34	Joback Method
dvisc	0.0033747	Pa×s	391.83	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=R249246&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