2-Carboxymethyl-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C6H8O5/c1-10-5(9)6(3-11-6)2-4(7)8/h2-3H2,1H3,(H,7,8)
InchiKey: NPLCGOZVEOVQGF-UHFFFAOYSA-N
Formula: C6H8O5
SMILES: COC(=O)C1(CC(=O)O)CO1
Mol. weight [g/mol]: 160.12

Physical Properties

Property code	Value	Unit	Source
gf	-530.88	kJ/mol	Joback Method
hf	-720.74	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	0.61		Crippen Method
logp	-0.597		Crippen Method
mcvol	105.290	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
rinpol	1180.00		NIST Webbook
tb	592.95	K	Joback Method
tc	790.67	K	Joback Method
tf	408.70	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.26	J/mol×K	592.95	Joback Method
cpg	273.93	J/mol×K	625.90	Joback Method
cpg	281.16	J/mol×K	658.86	Joback Method
cpg	288.05	J/mol×K	691.81	Joback Method
cpg	294.66	J/mol×K	724.76	Joback Method
cpg	301.10	J/mol×K	757.72	Joback Method
cpg	307.43	J/mol×K	790.67	Joback Method

Sources

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=R249157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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