2-(2-Methoxycarbonyl-ethyl)-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C8H12O5/c1-11-6(9)3-4-8(5-13-8)7(10)12-2/h3-5H2,1-2H3
InchiKey: MUENPMULFJSIGN-UHFFFAOYSA-N
Formula: C8H12O5
SMILES: COC(=O)CCC1(C(=O)OC)CO1
Mol. weight [g/mol]: 188.18

Physical Properties

Property code	Value	Unit	Source
gf	-482.22	kJ/mol	Joback Method
hf	-742.01	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	54.99	kJ/mol	Joback Method
log10ws	9.80e-03		Crippen Method
logp	-0.118		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1291.00		NIST Webbook
tb	568.95	K	Joback Method
tc	772.22	K	Joback Method
tf	392.65	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.59	J/mol×K	568.95	Joback Method
cpg	345.86	J/mol×K	602.83	Joback Method
cpg	356.52	J/mol×K	636.71	Joback Method
cpg	366.64	J/mol×K	670.58	Joback Method
cpg	376.31	J/mol×K	704.46	Joback Method
cpg	385.61	J/mol×K	738.34	Joback Method
cpg	394.61	J/mol×K	772.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249137&Units=SI

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