2-(4-Carboxy-butyl)-oxirane-2-carboxylic acid methyl ester

Inchi: InChI=1S/C9H14O5/c1-13-8(12)9(6-14-9)5-3-2-4-7(10)11/h2-6H2,1H3,(H,10,11)
InchiKey: IRLNAJWVPPQRSU-UHFFFAOYSA-N
Formula: C9H14O5
SMILES: COC(=O)C1(CCCCC(=O)O)CO1
Mol. weight [g/mol]: 202.20

Physical Properties

Property code	Value	Unit	Source
gf	-505.62	kJ/mol	Joback Method
hf	-782.66	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	71.48	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.573		Crippen Method
mcvol	147.560	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	661.59	K	Joback Method
tc	852.52	K	Joback Method
tf	442.51	K	Joback Method
vc	0.565	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.47	J/mol×K	661.59	Joback Method
cpg	416.70	J/mol×K	693.41	Joback Method
cpg	426.50	J/mol×K	725.23	Joback Method
cpg	435.96	J/mol×K	757.05	Joback Method
cpg	445.15	J/mol×K	788.88	Joback Method
cpg	454.16	J/mol×K	820.70	Joback Method
cpg	463.08	J/mol×K	852.52	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=R249142&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