Ethyl 5,6-Epoxyhexanoate

Inchi: InChI=1S/C8H14O3/c1-2-10-8(9)5-3-4-7-6-11-7/h7H,2-6H2,1H3
InchiKey: IMJURUKQBKWFLX-UHFFFAOYSA-N
Formula: C8H14O3
SMILES: CCOC(=O)CCCC1CO1
Mol. weight [g/mol]: 158.19

Physical Properties

Property code	Value	Unit	Source
gf	-242.81	kJ/mol	Joback Method
hf	-512.45	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	46.98	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.119		Crippen Method
mcvol	126.030	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1214.00		NIST Webbook
tb	492.42	K	Joback Method
tc	680.92	K	Joback Method
tf	296.59	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.49	J/mol×K	492.42	Joback Method
cpg	352.97	J/mol×K	649.50	Joback Method
cpg	342.43	J/mol×K	618.09	Joback Method
cpg	331.33	J/mol×K	586.67	Joback Method
cpg	319.66	J/mol×K	555.25	Joback Method
cpg	307.38	J/mol×K	523.84	Joback Method
cpg	362.97	J/mol×K	680.92	Joback Method
dvisc	0.0005168	Pa×s	492.42	Joback Method
dvisc	0.0006093	Pa×s	459.78	Joback Method

dvisc	0.0007368	Pa×s	427.14	Joback Method
dvisc	0.0009194	Pa×s	394.50	Joback Method
dvisc	0.0011940	Pa×s	361.87	Joback Method
dvisc	0.0016330	Pa×s	329.23	Joback Method
dvisc	0.0023929	Pa×s	296.59	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=R412716&Units=SI

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