3,3,3-Trifluoro-1,2-epoxypropane

Other names: Oxirane, 2-(trifluoromethyl)-
1,1,1-Trifluoro-2,3-epoxypropane
Inchi: InChI=1S/C3H3F3O/c4-3(5,6)2-1-7-2/h2H,1H2
InchiKey: AQZRARFZZMGLHL-UHFFFAOYSA-N
Formula: C3H3F3O
SMILES: FC(F)(F)C1CO1
Mol. weight [g/mol]: 112.05
CAS: 359-41-1

Physical Properties

Property code	Value	Unit	Source
gf	-632.58	kJ/mol	Joback Method
hf	-761.53	kJ/mol	Joback Method
hfus	11.47	kJ/mol	Joback Method
hvap	22.95	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.948		Crippen Method
mcvol	53.450	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
rinpol	508.00		NIST Webbook
tb	296.31	K	Joback Method
tc	457.06	K	Joback Method
tf	172.27	K	Joback Method
vc	0.225	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.75	J/mol×K	296.31	Joback Method
cpg	101.94	J/mol×K	323.10	Joback Method
cpg	109.59	J/mol×K	349.89	Joback Method
cpg	116.74	J/mol×K	376.68	Joback Method
cpg	123.41	J/mol×K	403.48	Joback Method
cpg	129.62	J/mol×K	430.27	Joback Method

cpg	135.39	J/mol×K	457.06	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=C359411&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