2-Isobutoxyethyl trifluroacetate

Inchi: InChI=1S/C8H13F3O3/c1-6(2)5-13-3-4-14-7(12)8(9,10)11/h6H,3-5H2,1-2H3
InchiKey: ORJIOJWJYOBTNO-UHFFFAOYSA-N
Formula: C8H13F3O3
SMILES: CC(C)COCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 214.18

Physical Properties

Property code	Value	Unit	Source
gf	-906.47	kJ/mol	Joback Method
hf	-1187.83	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	40.83	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.764		Crippen Method
mcvol	142.200	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	927.40		NIST Webbook
tb	475.29	K	Joback Method
tc	638.73	K	Joback Method
tf	263.50	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.72	J/mol×K	475.29	Joback Method
cpg	343.40	J/mol×K	502.53	Joback Method
cpg	354.61	J/mol×K	529.77	Joback Method
cpg	365.37	J/mol×K	557.01	Joback Method
cpg	375.67	J/mol×K	584.25	Joback Method
cpg	385.52	J/mol×K	611.49	Joback Method
cpg	394.94	J/mol×K	638.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188844&Units=SI
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

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