2-Isopentoxyethyl trifluoroacetate

Inchi: InChI=1S/C9H15F3O3/c1-7(2)3-4-14-5-6-15-8(13)9(10,11)12/h7H,3-6H2,1-2H3
InchiKey: UZIQAFXKDBUWMR-UHFFFAOYSA-N
Formula: C9H15F3O3
SMILES: CC(C)CCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 228.21

Physical Properties

Property code	Value	Unit	Source
gf	-898.05	kJ/mol	Joback Method
hf	-1208.47	kJ/mol	Joback Method
hfus	21.34	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	2.155		Crippen Method
mcvol	156.290	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1022.30		NIST Webbook
rinpol	1022.30		NIST Webbook
tb	498.17	K	Joback Method
tc	660.74	K	Joback Method
tf	274.77	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.95	J/mol×K	498.17	Joback Method
cpg	388.50	J/mol×K	525.27	Joback Method
cpg	400.54	J/mol×K	552.36	Joback Method
cpg	412.08	J/mol×K	579.46	Joback Method
cpg	423.13	J/mol×K	606.55	Joback Method
cpg	433.69	J/mol×K	633.65	Joback Method
cpg	443.77	J/mol×K	660.74	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=R188884&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