2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethyl trifluroacetate

InchI: InChI=1S/C14H25F3O6/c1-12(2)11-22-8-7-20-4-3-19-5-6-21-9-10-23-13(18)14(15,16)17
InchiKey: JCJADSYCGFXHKB-UHFFFAOYSA-N
Formula: C14H25F3O6
SMILES: CC(C)COCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-1170.95	kJ/mol	Joback Method
hf	-1708.33	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.814		Crippen Method
mcvol	244.350	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1704.70		NIST Webbook
tb	679.83	K	Joback Method
tc	843.87	K	Joback Method
tf	397.81	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.81	J/mol×K	679.83	Joback Method
cpg	727.16	J/mol×K	707.17	Joback Method
cpg	741.80	J/mol×K	734.51	Joback Method
cpg	755.74	J/mol×K	761.85	Joback Method
cpg	768.96	J/mol×K	789.19	Joback Method
cpg	781.46	J/mol×K	816.53	Joback Method
cpg	793.23	J/mol×K	843.87	Joback Method

Sources

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=R188488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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