2-(2-(2-Isopentoxy-ethoxy)-ethoxy)-ethyl trifluoroacetate

InchI: InChI=1S/C15H27F3O6/c1-13(2)3-4-20-5-6-21-7-8-22-9-10-23-11-12-24-14(19)15(16,17
InchiKey: YECGVPHJGUWBNM-UHFFFAOYSA-N
Formula: C15H27F3O6
SMILES: CC(C)CCOCCOCCOCCOCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-1162.53	kJ/mol	Joback Method
hf	-1728.97	kJ/mol	Joback Method
hfus	40.45	kJ/mol	Joback Method
hvap	63.64	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.204		Crippen Method
mcvol	258.440	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	1800.80		NIST Webbook
rinpol	1800.80		NIST Webbook
tb	702.71	K	Joback Method
tc	868.34	K	Joback Method
tf	409.08	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.82	J/mol×K	702.71	Joback Method
cpg	783.69	J/mol×K	730.32	Joback Method
cpg	798.80	J/mol×K	757.92	Joback Method
cpg	813.14	J/mol×K	785.53	Joback Method
cpg	826.71	J/mol×K	813.13	Joback Method
cpg	839.50	J/mol×K	840.74	Joback Method
cpg	851.51	J/mol×K	868.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188562&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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