2-[2-(2-Isopentoxyethoxy)ethoxy]ethyl trifluoroacetate

Inchi: InChI=1S/C13H23F3O5/c1-11(2)3-4-18-5-6-19-7-8-20-9-10-21-12(17)13(14,15)16/h11H,

InchiKey: UCQNZHPFIAQFDQ-UHFFFAOYSA-N

Formula: C13H23F3O5

SMILES: CC(C)CCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]: 316.31

Physical Properties

Property code	Value	Unit	Source
gf	-1074.37	kJ/mol	Joback Method
hf	-1555.47	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	56.78	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	2.188		Crippen Method
mcvol	224.390	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	1548.00		NIST Webbook
tb	634.53	K	Joback Method
tc	796.36	K	Joback Method
tf	364.31	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.24	J/mol×K	634.53	Joback Method
cpg	643.15	J/mol×K	661.50	Joback Method
cpg	657.43	J/mol×K	688.47	Joback Method
cpg	671.06	J/mol×K	715.45	Joback Method
cpg	684.07	J/mol×K	742.42	Joback Method
cpg	696.43	J/mol×K	769.39	Joback Method
cpg	708.16	J/mol×K	796.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188597&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