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

Inchi: InChI=1S/C12H21F3O5/c1-10(2)9-19-6-5-17-3-4-18-7-8-20-11(16)12(13,14)15/h10H,3-9

InchiKey: ZQJREBJWKAQRLY-UHFFFAOYSA-N

Formula: C12H21F3O5

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

Mol. weight [g/mol]: 302.29

Physical Properties

Property code	Value	Unit	Source
gf	-1082.79	kJ/mol	Joback Method
hf	-1534.83	kJ/mol	Joback Method
hfus	31.49	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.798		Crippen Method
mcvol	210.300	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	1451.00		NIST Webbook
rinpol	1451.00		NIST Webbook
tb	611.65	K	Joback Method
tc	773.19	K	Joback Method
tf	353.04	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.52	J/mol×K	611.65	Joback Method
cpg	589.84	J/mol×K	638.57	Joback Method
cpg	603.58	J/mol×K	665.50	Joback Method
cpg	616.72	J/mol×K	692.42	Joback Method
cpg	629.27	J/mol×K	719.34	Joback Method
cpg	641.23	J/mol×K	746.26	Joback Method
cpg	652.60	J/mol×K	773.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188517&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