2-(2-(2-(2-(2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethox trifluroacetate

InchI: InChI=1S/C22H41F3O10/c1-20(2)19-34-16-15-32-12-11-30-8-7-28-4-3-27-5-6-29-9-10-3

InchiKey: ONZPATNLHYTNRN-UHFFFAOYSA-N

Formula: C22H41F3O10

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

Mol. weight [g/mol]: 522.55

Physical Properties

Property code	Value	Unit	Source
gf	-1523.59	kJ/mol	Joback Method
hf	-2402.33	kJ/mol	Joback Method
hfus	63.33	kJ/mol	Joback Method
hvap	88.87	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.881		Crippen Method
mcvol	380.550	ml/mol	McGowan Method
pc	803.42	kPa	Joback Method
rinpol	2760.30		NIST Webbook
rinpol	2760.30		NIST Webbook
tb	952.55	K	Joback Method
tc	1184.58	K	Joback Method
tf	576.89	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1311.44	J/mol×K	952.55	Joback Method
cpg	1329.36	J/mol×K	991.22	Joback Method
cpg	1344.69	J/mol×K	1029.89	Joback Method
cpg	1357.37	J/mol×K	1068.56	Joback Method
cpg	1367.35	J/mol×K	1107.23	Joback Method
cpg	1374.57	J/mol×K	1145.90	Joback Method
cpg	1378.97	J/mol×K	1184.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R187836&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

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