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

Inchi: InChI=1S/C20H37F3O9/c1-18(2)17-31-14-13-29-10-9-27-6-5-25-3-4-26-7-8-28-11-12-30

InchiKey: LSAYFZNCCAGWAY-UHFFFAOYSA-N

Formula: C20H37F3O9

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

Mol. weight [g/mol]: 478.50

Physical Properties

Property code	Value	Unit	Source
gf	-1435.43	kJ/mol	Joback Method
hf	-2228.83	kJ/mol	Joback Method
hfus	56.96	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.864		Crippen Method
mcvol	346.500	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	2498.10		NIST Webbook
tb	884.37	K	Joback Method
tc	1087.19	K	Joback Method
tf	532.12	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.63	J/mol×K	884.37	Joback Method
cpg	1175.42	J/mol×K	918.17	Joback Method
cpg	1191.52	J/mol×K	951.98	Joback Method
cpg	1205.87	J/mol×K	985.78	Joback Method
cpg	1218.46	J/mol×K	1019.59	Joback Method
cpg	1229.25	J/mol×K	1053.39	Joback Method
cpg	1238.21	J/mol×K	1087.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R187970&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