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

InchI: InChI=1S/C16H29F3O7/c1-14(2)13-25-10-9-23-6-5-21-3-4-22-7-8-24-11-12-26-15(20)16

InchiKey: RTHKMWVSDJTRCZ-UHFFFAOYSA-N

Formula: C16H29F3O7

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

Mol. weight [g/mol]: 390.39

Physical Properties

Property code	Value	Unit	Source
gf	-1259.11	kJ/mol	Joback Method
hf	-1881.83	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	1.831		Crippen Method
mcvol	278.400	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	1973.10		NIST Webbook
rinpol	1973.10		NIST Webbook
tb	748.01	K	Joback Method
tc	918.72	K	Joback Method
tf	442.58	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.56	J/mol×K	748.01	Joback Method
cpg	871.84	J/mol×K	776.46	Joback Method
cpg	887.24	J/mol×K	804.91	Joback Method
cpg	901.73	J/mol×K	833.37	Joback Method
cpg	915.31	J/mol×K	861.82	Joback Method
cpg	927.98	J/mol×K	890.27	Joback Method
cpg	939.71	J/mol×K	918.72	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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