

2-(2-(2-(2-(2-Isobutoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethyl trifluoroacetate

InChI:

InChI=1S/C18H33F3O8/c1-16(2)15-28-12-11-26-8-7-24-4-3-23-5-6-25-9-10-27-13-14-29

InchiKey:

WKIGYMSBMMKYGL-UHFFFAOYSA-N

Formula:

C18H33F3O8

SMILES:

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

Mol. weight [g/mol]:

434.44

Physical Properties

Property code	Value	Unit	Source
gf	-1347.27	kJ/mol	Joback Method
hf	-2055.33	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	75.14	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.848		Crippen Method
mcvol	312.450	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2233.10		NIST Webbook
rinpol	2233.10		NIST Webbook
tb	816.19	K	Joback Method
tc	999.26	K	Joback Method
tf	487.35	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.88	J/mol×K	816.19	Joback Method
cpg	1022.02	J/mol×K	846.70	Joback Method
cpg	1037.96	J/mol×K	877.21	Joback Method
cpg	1052.69	J/mol×K	907.72	Joback Method
cpg	1066.20	J/mol×K	938.24	Joback Method
cpg	1078.46	J/mol×K	968.75	Joback Method
cpg	1089.45	J/mol×K	999.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188131&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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