

2-(2-(2-(2-(2-Butoxy-ethoxy)-ethoxy)-ethoxy)-ethoxy)-ethoxytrifluoroacetate

InChI:InChI=1S/C18H33F3O8/c1-2-3-4-23-5-6-24-7-8-25-9-10-26-11-12-27-13-14-28-15-16-29-30-31-32-33-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100

InchiKey:OBYZGWRUDXNGIE-UHFFFAOYSA-N

Formula:C18H33F3O8

SMILES:CCCCOCCOCCOCCOCCOCCOCCOC(=O)C(F)(F)F

Mol. weight [g/mol]:434.44

Physical Properties

Property code	Value	Unit	Source
gf	-1344.83	kJ/mol	Joback Method
hf	-2050.05	kJ/mol	Joback Method
hfus	54.12	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-1.41		Crippen Method
logp	1.992		Crippen Method
mcvol	312.450	ml/mol	McGowan Method
pc	1028.60	kPa	Joback Method
rinpol	2268.60		NIST Webbook
tb	816.63	K	Joback Method
tc	999.92	K	Joback Method
tf	502.35	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.39	J/mol×K	816.63	Joback Method
cpg	1021.54	J/mol×K	847.18	Joback Method
cpg	1037.51	J/mol×K	877.73	Joback Method
cpg	1052.27	J/mol×K	908.28	Joback Method
cpg	1065.81	J/mol×K	938.83	Joback Method
cpg	1078.10	J/mol×K	969.38	Joback Method
cpg	1089.14	J/mol×K	999.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188082&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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