2-(2-(2-Pentoxy-ethoxy)-ethoxy)-ethoxy)-ethyl trifluoroacetate

Inchi: InChI=1S/C15H27F3O6/c1-2-3-4-5-20-6-7-21-8-9-22-10-11-23-12-13-24-14(19)15(16,17

InchiKey: XQORWRGLWKDJJV-UHFFFAOYSA-N

Formula: C15H27F3O6

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

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-1160.09	kJ/mol	Joback Method
hf	-1723.69	kJ/mol	Joback Method
hfus	43.97	kJ/mol	Joback Method
hvap	64.03	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.349		Crippen Method
mcvol	258.440	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1836.20		NIST Webbook
rinpol	1836.20		NIST Webbook
tb	703.15	K	Joback Method
tc	867.58	K	Joback Method
tf	424.08	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.35	J/mol×K	703.15	Joback Method
cpg	783.09	J/mol×K	730.56	Joback Method
cpg	798.08	J/mol×K	757.96	Joback Method
cpg	812.31	J/mol×K	785.37	Joback Method
cpg	825.79	J/mol×K	812.77	Joback Method
cpg	838.51	J/mol×K	840.18	Joback Method
cpg	850.47	J/mol×K	867.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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