2-[2-[2-[2-(2,2,2-Trifluoroacetyl)oxyethoxy]ethoxy]ethoxy]ethoxy] 2,2,2-trifluoroacetate

Other names: Tetraethylene glycol, bis(trifluoroacetate)
14,14,14-Trifluoro-13-oxo-3,6,9,12-tetraoxatetradec-1-yl trifluoroacetate

Inchi: InChI=1S/C12H16F6O7/c13-11(14,15)9(19)24-7-5-22-3-1-21-2-4-23-6-8-25-10(20)12(16

InchiKey: GUPRYWKQXRVSDN-UHFFFAOYSA-N

Formula: C12H16F6O7

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

Mol. weight [g/mol]: 386.24

Physical Properties

Property code	Value	Unit	Source
gf	-1895.86	kJ/mol	Joback Method
hf	-2371.43	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	60.35	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.247		Crippen Method
mcvol	223.050	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	1467.70		NIST Webbook
tb	682.96	K	Joback Method
tc	844.76	K	Joback Method
tf	444.39	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.25	J/mol×K	682.96	Joback Method
cpg	663.44	J/mol×K	709.93	Joback Method
cpg	674.99	J/mol×K	736.89	Joback Method
cpg	685.90	J/mol×K	763.86	Joback Method
cpg	696.17	J/mol×K	790.82	Joback Method
cpg	705.80	J/mol×K	817.79	Joback Method
cpg	714.79	J/mol×K	844.76	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=U351943&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

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