

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

Other names: Triethylene glycol bis(trifluoroacetate)
2,2,2-trifluoroacetate 11,11,11-Trifluoro-10-oxo-3,6,9-trioxaundec-1-yl trifluoroacetate

Inchi: InChI=1S/C10H12F6O6/c11-9(12,13)7(17)21-5-3-19-1-2-20-4-6-22-8(18)10(14,15)16/h1

InchiKey: AIYYCLMMVJJPJB-UHFFFAOYSA-N

Formula: C10H12F6O6

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

Mol. weight [g/mol]: 342.19

Physical Properties

Property code	Value	Unit	Source
gf	-1807.70	kJ/mol	Joback Method
hf	-2197.93	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	53.49	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.231		Crippen Method
mcvol	189.000	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1234.20		NIST Webbook
tb	614.78	K	Joback Method
tc	772.80	K	Joback Method
tf	399.62	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.27	J/molxK	614.78	Joback Method
cpg	533.34	J/molxK	641.12	Joback Method
cpg	543.87	J/molxK	667.45	Joback Method
cpg	553.86	J/molxK	693.79	Joback Method
cpg	563.33	J/molxK	720.13	Joback Method
cpg	572.27	J/molxK	746.47	Joback Method
cpg	580.70	J/molxK	772.80	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=U351899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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