

2-[2-[2-(2-Ethoxyethoxy)ethoxy]ethoxy]ethyl 2,2,2-trifluoroacetate

Other names: Tetraethylene glycol monoethyl ether, trifluoroacetate
3,6,9,12-Tetraoxatetradec-1-yl trifluoroacetate

Inchi: InChI=1S/C12H21F3O6/c1-2-17-3-4-18-5-6-19-7-8-20-9-10-21-11(16)12(13,14)15/h2-10

InchiKey: QLHDTTPYYQAFDJ-UHFFFAOYSA-N

Formula: C12H21F3O6

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

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-1185.35	kJ/mol	Joback Method
hf	-1661.77	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	1.178		Crippen Method
mcvol	216.170	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1532.50		NIST Webbook
rinpol	1532.50		NIST Webbook
tb	634.51	K	Joback Method
tc	794.90	K	Joback Method
tf	390.27	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.15	J/mol×K	634.51	Joback Method
cpg	617.16	J/mol×K	661.24	Joback Method
cpg	630.59	J/mol×K	687.97	Joback Method
cpg	643.44	J/mol×K	714.70	Joback Method
cpg	655.71	J/mol×K	741.44	Joback Method
cpg	667.38	J/mol×K	768.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351931&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
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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