

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

Other names: Tetraethylene glycol monobutyl ether, trifluoroacetate
3,6,9,12-Tetraoxahexadec-1-yl trifluoroacetate

Inchi: InChI=1S/C14H25F3O6/c1-2-3-4-19-5-6-20-7-8-21-9-10-22-11-12-23-13(18)14(15,16)17

InchiKey: ZTOUDZGTXQOXCW-UHFFFAOYSA-N

Formula: C14H25F3O6

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

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-1168.51	kJ/mol	Joback Method
hf	-1703.05	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.958		Crippen Method
mcvol	244.350	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1735.10		NIST Webbook
rinpol	1735.10		NIST Webbook
rinpol	1703.10		NIST Webbook
rinpol	1703.10		NIST Webbook
tb	680.27	K	Joback Method
tc	842.85	K	Joback Method
tf	412.81	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.36	J/mol×K	680.27	Joback Method
cpg	726.54	J/mol×K	707.37	Joback Method
cpg	741.04	J/mol×K	734.46	Joback Method
cpg	754.85	J/mol×K	761.56	Joback Method

cpg	767.96	J/mol×K	788.66	Joback Method
cpg	780.37	J/mol×K	815.76	Joback Method
cpg	792.07	J/mol×K	842.85	Joback Method

Sources

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=U351937&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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