2-[2-[2-(2-Butoxyethoxy)ethoxy]ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate

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

Inchi: InChI=1S/C15H25F5O6/c1-2-3-4-22-5-6-23-7-8-24-9-10-25-11-12-26-13(21)14(16,17)15

InchiKey: COFNBSPQYZUHQI-UHFFFAOYSA-N

Formula: C15H25F5O6

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

Mol. weight [g/mol]: 396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1546.87	kJ/mol	Joback Method
hf	-2124.66	kJ/mol	Joback Method
hfus	42.72	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.594		Crippen Method
mcvol	261.980	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	1703.30		NIST Webbook
tb	698.46	K	Joback Method
tc	860.21	K	Joback Method
tf	427.68	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.15	J/mol×K	698.46	Joback Method
cpg	800.34	J/mol×K	725.42	Joback Method
cpg	814.77	J/mol×K	752.38	Joback Method
cpg	828.45	J/mol×K	779.34	Joback Method
cpg	841.39	J/mol×K	806.30	Joback Method
cpg	853.59	J/mol×K	833.25	Joback Method
cpg	865.05	J/mol×K	860.21	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=U351989&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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