2-[2-[2-(2-Butoxyethoxy)ethoxy]ethoxy]ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

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

Inchi: InChI=1S/C16H25F7O6/c1-2-3-4-25-5-6-26-7-8-27-9-10-28-11-12-29-13(24)14(17,18)15

InchiKey: KBVASKWGNYMXBL-UHFFFAOYSA-N

Formula: C16H25F7O6

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

Mol. weight [g/mol]: 446.35

Physical Properties

Property code	Value	Unit	Source
gf	-1925.23	kJ/mol	Joback Method
hf	-2546.27	kJ/mol	Joback Method
hfus	44.05	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.229		Crippen Method
mcvol	279.610	ml/mol	McGowan Method
pc	1086.35	kPa	Joback Method
rinpol	1732.40		NIST Webbook
rinpol	1732.40		NIST Webbook
tb	716.65	K	Joback Method
tc	879.16	K	Joback Method
tf	442.55	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.38	J/mol×K	716.65	Joback Method
cpg	874.62	J/mol×K	743.74	Joback Method
cpg	889.02	J/mol×K	770.82	Joback Method
cpg	902.62	J/mol×K	797.91	Joback Method
cpg	915.42	J/mol×K	824.99	Joback Method
cpg	927.44	J/mol×K	852.08	Joback Method

cpg	938.71	J/mol×K	879.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352021&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