2-[2-[2-(2,2,3,3,4,4,4-Heptafluorobutanoyl)oxyetho
2,2,3,3,4,4,4-heptafluorobutanate

Other names:	11,11,12,12,13,13,13-Heptafluoro-10-oxo-3,6,9-trioxatridec-1-yl heptafluorobutyrate Triethylene glycol, bis(heptafluorobutyrate)
Inchi:	InChI=1S/C14H12F14O6/c15-9(16,11(19,20)13(23,24)25)7(29)33-5-3-31-1-2-32-4-6-34-8
InchiKey:	RMENOZLMYVQJGN-UHFFFAOYSA-N
Formula:	C14H12F14O6
SMILES:	O=C(OCCOCCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	542.22

Physical Properties

Property code	Value	Unit	Source
gf	-3321.14	kJ/mol	Joback Method
hf	-3884.37	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.772		Crippen Method
mcvol	259.520	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	1324.50		NIST Webbook
tb	687.54	K	Joback Method
tc	842.69	K	Joback Method
tf	459.10	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.65	J/mol×K	687.54	Joback Method
cpg	816.29	J/mol×K	713.40	Joback Method
cpg	827.12	J/mol×K	739.26	Joback Method
cpg	837.19	J/mol×K	765.11	Joback Method
cpg	846.55	J/mol×K	790.97	Joback Method
cpg	855.24	J/mol×K	816.83	Joback Method
cpg	863.30	J/mol×K	842.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352030&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

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