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

Other names: Triethylene glycol monobutyl ether, heptafluorobutyrate

3,6,9-Trioxatridec-1-yl heptafluorobutyrate

Inchi: InChI=1S/C14H21F7O5/c1-2-3-4-23-5-6-24-7-8-25-9-10-26-11(22)12(15,16)13(17,18)14

InchiKey: BZTFUNZLKSUPGB-UHFFFAOYSA-N

Formula: C14H21F7O5

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

Mol. weight [g/mol]: 402.30

Physical Properties

Property code	Value	Unit	Source
gf	-1837.07	kJ/mol	Joback Method
hf	-2372.77	kJ/mol	Joback Method
hfus	37.68	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	3.212		Crippen Method
mcvol	245.560	ml/mol	McGowan Method
pc	1253.03	kPa	Joback Method
rinpol	1488.80		NIST Webbook
tb	648.47	K	Joback Method
tc	802.84	K	Joback Method
tf	397.78	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.84	J/mol×K	648.47	Joback Method
cpg	733.11	J/mol×K	674.20	Joback Method
cpg	746.66	J/mol×K	699.93	Joback Method
cpg	759.53	J/mol×K	725.65	Joback Method
cpg	771.72	J/mol×K	751.38	Joback Method
cpg	783.25	J/mol×K	777.11	Joback Method
cpg	794.15	J/mol×K	802.84	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=U352020&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