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

Other names: Triethylene glycol monomethyl ether, heptafluorobutyrate
3,6,9-Trioxadeca-1-yl heptafluorobutyrate

Inchi: InChI=1S/C11H15F7O5/c1-20-2-3-21-4-5-22-6-7-23-8(19)9(12,13)10(14,15)11(16,17)18/

InchiKey: UHMSQURMLHELID-UHFFFAOYSA-N

Formula: C11H15F7O5

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

Mol. weight [g/mol]: 360.22

Physical Properties

Property code	Value	Unit	Source
gf	-1862.33	kJ/mol	Joback Method
hf	-2310.85	kJ/mol	Joback Method
hfus	29.92	kJ/mol	Joback Method
hvap	46.86	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	2.042		Crippen Method
mcvol	203.290	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	1274.80		NIST Webbook
rinpol	1274.80		NIST Webbook
tb	579.83	K	Joback Method
tc	730.54	K	Joback Method
tf	363.97	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.54	J/mol×K	579.83	Joback Method
cpg	575.18	J/mol×K	604.95	Joback Method
cpg	587.21	J/mol×K	630.07	Joback Method
cpg	598.65	J/mol×K	655.18	Joback Method
cpg	609.52	J/mol×K	680.30	Joback Method
cpg	619.83	J/mol×K	705.42	Joback Method

cpg	629.60	J/mol×K	730.54	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=U352005&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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