

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

Other names:

Tetraethylene glycol monomethyl ether, heptafluorobutyrate

3,6,9,12-Tetraoxatridec-1-yl heptafluorobutyrate

Inchi:

InChI=1S/C13H19F7O6/c1-22-2-3-23-4-5-24-6-7-25-8-9-26-10(21)11(14,15)12(16,17)13

InchiKey:

SAKWEGWATBORGR-UHFFFAOYSA-N

Formula:

C13H19F7O6

SMILES:

COCCOCCOCCOCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]:

404.28

Physical Properties

Property code	Value	Unit	Source
gf	-1950.49	kJ/mol	Joback Method
hf	-2484.35	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	2.059		Crippen Method
mcvol	237.340	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	1515.40		NIST Webbook
tb	648.01	K	Joback Method
tc	802.67	K	Joback Method
tf	408.74	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.78	J/molxK	648.01	Joback Method
cpg	707.39	J/molxK	673.79	Joback Method
cpg	720.33	J/molxK	699.56	Joback Method
cpg	732.60	J/molxK	725.34	Joback Method
cpg	744.23	J/molxK	751.12	Joback Method
cpg	755.21	J/molxK	776.89	Joback Method
cpg	765.58	J/molxK	802.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U352006&Units=SI

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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