

2-[2-[2-[2-(2-Methoxyethoxy)ethoxy]ethoxy]ethoxy]ethoxy

Other names: 2,2,3,3,4,4,4-heptafluorobutanoate
Pentaethylene glycol monomethyl ether, heptafluorobutyrate
3,6,9,12,15-Heptaaoxahexadec-1-yl heptafluorobutyrate

Inchi: InChI=1S/C15H23F7O7/c1-24-2-3-25-4-5-26-6-7-27-8-9-28-10-11-29-12(23)13(16,17)14

InchiKey: HSGCBGFZWVAMCH-UHFFFAOYSA-N

Formula: C15H23F7O7

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

Mol. weight [g/mol]: 448.33

Physical Properties

Property code	Value	Unit	Source
gf	-2038.65	kJ/mol	Joback Method
hf	-2657.85	kJ/mol	Joback Method
hfus	42.65	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	2.075		Crippen Method
mcvol	271.390	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	1763.90		NIST Webbook
rinpol	1763.90		NIST Webbook
tb	716.19	K	Joback Method
tc	878.79	K	Joback Method
tf	453.51	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.55	J/mol×K	716.19	Joback Method
cpg	847.18	J/mol×K	743.29	Joback Method
cpg	861.00	J/mol×K	770.39	Joback Method
cpg	874.02	J/mol×K	797.49	Joback Method
cpg	886.26	J/mol×K	824.59	Joback Method
cpg	897.72	J/mol×K	851.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352007&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

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