

2-(2-Butoxyethoxy)ethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names:

Diethylene glycol butyl ether, heptafluorobutyrate

3,6-Dioxaodec-1-yl heptafluorobutyrate

Inchi: InChI=1S/C12H17F7O4/c1-2-3-4-21-5-6-22-7-8-23-9(20)10(13,14)11(15,16)12(17,18)19

InchiKey: RGLAKFJGHIKBNF-UHFFFAOYSA-N

Formula: C12H17F7O4

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

Mol. weight [g/mol]: 358.25

Physical Properties

Property code	Value	Unit	Source
gf	-1748.91	kJ/mol	Joback Method
hf	-2199.27	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.196		Crippen Method
mcvol	211.510	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	1248.50		NIST Webbook
rinpol	1248.50		NIST Webbook
tb	580.29	K	Joback Method
tc	730.53	K	Joback Method
tf	353.01	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.51	J/molxK	580.29	Joback Method
cpg	598.91	J/molxK	605.33	Joback Method
cpg	611.65	J/molxK	630.37	Joback Method
cpg	623.76	J/molxK	655.41	Joback Method
cpg	635.25	J/molxK	680.45	Joback Method
cpg	646.16	J/molxK	705.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352019&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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