2-Methyl-1,4-butanediol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C13H10F14O4/c1-5(4-31-7(29)9(16,17)11(20,21)13(25,26)27)2-3-30-6(28)8(14

InchiKey: DSSSASSXAGZFOT-UHFFFAOYSA-N

Formula: C13H10F14O4

SMILES: CC(CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F)COC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 496.19

Physical Properties

Property code	Value	Unit	Source
gf	-3122.00	kJ/mol	Joback Method
hf	-3604.57	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	43.24	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.765		Crippen Method
mcvol	233.690	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	619.38	K	Joback Method
tc	765.91	K	Joback Method
tf	388.37	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.71	J/mol×K	619.38	Joback Method
cpg	710.41	J/mol×K	643.80	Joback Method
cpg	721.31	J/mol×K	668.22	Joback Method
cpg	731.45	J/mol×K	692.64	Joback Method
cpg	740.87	J/mol×K	717.06	Joback Method
cpg	749.64	J/mol×K	741.49	Joback Method
cpg	757.78	J/mol×K	765.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376239&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