1,4-Dioxane-2,3-diol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C12H6F14O6/c13-7(14,9(17,18)11(21,22)23)5(27)31-3-4(30-2-1-29-3)32-6(28)
InchiKey: ORCFXVKIIBFIHK-UHFFFAOYSA-N
Formula: C12H6F14O6
SMILES: O=C(OC1OCCOC1OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 512.15

Physical Properties

Property code	Value	Unit	Source
gf	-3283.48	kJ/mol	Joback Method
hf	-3808.67	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	50.54	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.438		Crippen Method
mcvol	220.480	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	1075.00		NIST Webbook
tb	665.72	K	Joback Method
tc	828.04	K	Joback Method
tf	448.38	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.78	J/mol×K	665.72	Joback Method
cpg	714.16	J/mol×K	692.77	Joback Method
cpg	724.62	J/mol×K	719.83	Joback Method
cpg	734.21	J/mol×K	746.88	Joback Method
cpg	742.98	J/mol×K	773.93	Joback Method
cpg	750.99	J/mol×K	800.99	Joback Method
cpg	758.30	J/mol×K	828.04	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375754&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
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