2-Butene-1,4-diol, bis(heptafluorobutyrate)

Inchi: InChI=1S/C12H6F14O4/c13-7(14,9(17,18)11(21,22)23)5(27)29-3-1-2-4-30-6(28)8(15,16)
InchiKey: VMCQJLHZMCISBF-OWOJBTEDSA-N
Formula: C12H6F14O4
SMILES: O=C(OCC=CCOC(=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]: 480.15

Physical Properties

Property code	Value	Unit	Source
gf	-3047.76	kJ/mol	Joback Method
hf	-3461.43	kJ/mol	Joback Method
hfus	31.25	kJ/mol	Joback Method
hvap	41.36	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.295		Crippen Method
mcvol	215.300	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	1046.00		NIST Webbook
tb	601.10	K	Joback Method
tc	747.75	K	Joback Method
tf	387.02	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.52	J/mol×K	601.10	Joback Method
cpg	638.09	J/mol×K	625.54	Joback Method
cpg	647.87	J/mol×K	649.98	Joback Method
cpg	656.91	J/mol×K	674.42	Joback Method
cpg	665.26	J/mol×K	698.87	Joback Method
cpg	672.97	J/mol×K	723.31	Joback Method
cpg	680.09	J/mol×K	747.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375873&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

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