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

Inchi: InChI=1S/C10H6F10O4/c11-7(12,9(15,16)17)5(21)23-3-1-2-4-24-6(22)8(13,14)10(18,19)
InchiKey: ILPMBAWPVMKWRZ-OWOJBTEDSA-N
Formula: C10H6F10O4
SMILES: O=C(OCC=CCOC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 380.14

Physical Properties

Property code	Value	Unit	Source
gf	-2291.04	kJ/mol	Joback Method
hf	-2618.21	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	42.77	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.024		Crippen Method
mcvol	180.040	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	964.00		NIST Webbook
tb	564.72	K	Joback Method
tc	717.20	K	Joback Method
tf	357.28	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.56	J/mol×K	564.72	Joback Method
cpg	501.80	J/mol×K	590.13	Joback Method
cpg	511.34	J/mol×K	615.55	Joback Method
cpg	520.23	J/mol×K	640.96	Joback Method
cpg	528.49	J/mol×K	666.37	Joback Method
cpg	536.16	J/mol×K	691.79	Joback Method
cpg	543.29	J/mol×K	717.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375874&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