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

Inchi: InChI=1S/C11H10F10O4/c1-5(4-25-7(23)9(14,15)11(19,20)21)2-3-24-6(22)8(12,13)10(1
InchiKey: QYJMOSQGRXNUBG-UHFFFAOYSA-N
Formula: C11H10F10O4
SMILES: CC(CCOC(=O)C(F)(F)C(F)(F)F)COC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 396.18

Physical Properties

Property code	Value	Unit	Source
gf	-2365.28	kJ/mol	Joback Method
hf	-2761.35	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	44.65	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.494		Crippen Method
mcvol	198.430	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	1017.00		NIST Webbook
rinpol	1017.00		NIST Webbook
tb	583.00	K	Joback Method
tc	733.40	K	Joback Method
tf	358.63	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.54	J/mol×K	583.00	Joback Method
cpg	570.99	J/mol×K	608.07	Joback Method
cpg	581.75	J/mol×K	633.13	Joback Method
cpg	591.83	J/mol×K	658.20	Joback Method
cpg	601.28	J/mol×K	683.26	Joback Method
cpg	610.12	J/mol×K	708.33	Joback Method
cpg	618.39	J/mol×K	733.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376240&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