1,2-Propanediol, bis(pentafluoropropionate)

Inchi: InChI=1S/C9H6F10O4/c1-3(23-5(21)7(12,13)9(17,18)19)2-22-4(20)6(10,11)8(14,15)16/h
InchiKey: USYCVUCKLPWGPU-UHFFFAOYSA-N
Formula: C9H6F10O4
SMILES: CC(COC(=O)C(F)(F)C(F)(F)F)OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 368.13

Physical Properties

Property code	Value	Unit	Source
gf	-2382.12	kJ/mol	Joback Method
hf	-2720.07	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.856		Crippen Method
mcvol	170.250	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	907.00		NIST Webbook
tb	537.24	K	Joback Method
tc	686.73	K	Joback Method
tf	336.09	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.16	J/mol×K	537.24	Joback Method
cpg	474.62	J/mol×K	562.15	Joback Method
cpg	484.40	J/mol×K	587.07	Joback Method
cpg	493.55	J/mol×K	611.98	Joback Method
cpg	502.10	J/mol×K	636.90	Joback Method
cpg	510.06	J/mol×K	661.81	Joback Method
cpg	517.48	J/mol×K	686.73	Joback Method

Sources

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=U375546&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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