1,1,1-Tris(hydroxymethyl)propane, tri(pentafluoropropionate)

Inchi: InChI=1S/C15H11F15O6/c1-2-9(3-34-6(31)10(16,17)13(22,23)24,4-35-7(32)11(18,19)14
InchiKey: HBURXPQVCDTQEW-UHFFFAOYSA-N
Formula: C15H11F15O6
SMILES: CCC(COC(=O)C(F)(F)C(F)(F)F)(COC(=O)C(F)(F)C(F)(F)F)COC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 572.22

Physical Properties

Property code	Value	Unit	Source
gf	-3528.61	kJ/mol	Joback Method
hf	-4090.23	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	55.12	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.605		Crippen Method
mcvol	271.080	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	1117.00		NIST Webbook
tb	737.91	K	Joback Method
tc	903.66	K	Joback Method
tf	501.08	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.72	J/mol×K	737.91	Joback Method
cpg	869.32	J/mol×K	765.53	Joback Method
cpg	879.06	J/mol×K	793.16	Joback Method
cpg	888.02	J/mol×K	820.78	Joback Method
cpg	896.27	J/mol×K	848.41	Joback Method
cpg	903.89	J/mol×K	876.03	Joback Method
cpg	910.93	J/mol×K	903.66	Joback Method

Sources

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=U374841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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