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

Inchi: InChI=1S/C18H11F21O6/c1-2-9(3-43-6(40)10(19,20)13(25,26)16(31,32)33,4-44-7(41)11
InchiKey: IDAYENACLZKAEB-UHFFFAOYSA-N
Formula: C18H11F21O6
SMILES: CCC(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)(COC(=O)C(F)(F)C(F)(F)C(F)(F)F)COC(=O)C(F)(
Mol. weight [g/mol]: 722.24

Physical Properties

Property code	Value	Unit	Source
gf	-4663.69	kJ/mol	Joback Method
hf	-5355.06	kJ/mol	Joback Method
hfus	41.28	kJ/mol	Joback Method
hvap	53.01	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.511		Crippen Method
mcvol	323.970	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
tb	792.48	K	Joback Method
tc	976.36	K	Joback Method
tf	545.69	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.14	J/mol×K	792.48	Joback Method
cpg	1085.16	J/mol×K	823.13	Joback Method
cpg	1095.18	J/mol×K	853.77	Joback Method
cpg	1104.33	J/mol×K	884.42	Joback Method
cpg	1112.78	J/mol×K	915.07	Joback Method
cpg	1120.66	J/mol×K	945.72	Joback Method
cpg	1128.12	J/mol×K	976.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374307&Units=SI

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