L-Threitol, tetrakis(trifluoroacetate)

Inchi: InChI=1S/C12H6F12O8/c13-9(14,15)5(25)29-1-3(31-7(27)11(19,20)21)4(32-8(28)12(22,2

InchiKey: SIWZLDBXSQMWPJ-UHFFFAOYSA-N

Formula: C12H6F12O8

SMILES: O=C(OCC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 506.15

Physical Properties

Property code	Value	Unit	Source
gf	-3216.76	kJ/mol	Joback Method
hf	-3669.09	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.146		Crippen Method
mcvol	230.940	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	1026.70		NIST Webbook
tb	756.56	K	Joback Method
tc	927.46	K	Joback Method
tf	500.40	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.26	J/mol×K	756.56	Joback Method
cpg	716.89	J/mol×K	785.04	Joback Method
cpg	724.78	J/mol×K	813.53	Joback Method
cpg	731.96	J/mol×K	842.01	Joback Method
cpg	738.46	J/mol×K	870.49	Joback Method
cpg	744.31	J/mol×K	898.97	Joback Method
cpg	749.54	J/mol×K	927.46	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=U380213&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