Dulcitol, hexakis(trifluoroacetate)

Inchi: InChI=1S/C18H8F18O12/c19-13(20,21)7(37)43-1-3(45-9(39)15(25,26)27)5(47-11(41)17(
InchiKey: KHPSGAMQGNMDJO-UHFFFAOYSA-N
Formula: C18H8F18O12
SMILES: O=C(OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F
Mol. weight [g/mol]: 758.22

Physical Properties

Property code	Value	Unit	Source
gf	-4802.14	kJ/mol	Joback Method
hf	-5487.25	kJ/mol	Joback Method
hfus	55.96	kJ/mol	Joback Method
hvap	86.56	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.094		Crippen Method
mcvol	340.980	ml/mol	McGowan Method
pc	899.64	kPa	Joback Method
rinpol	1130.20		NIST Webbook
tb	1034.70	K	Joback Method
tc	1325.15	K	Joback Method
tf	690.72	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.87	J/mol×K	1034.70	Joback Method
cpg	1142.91	J/mol×K	1083.11	Joback Method
cpg	1147.19	J/mol×K	1131.52	Joback Method
cpg	1149.93	J/mol×K	1179.92	Joback Method
cpg	1151.37	J/mol×K	1228.33	Joback Method
cpg	1151.75	J/mol×K	1276.74	Joback Method
cpg	1151.32	J/mol×K	1325.15	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=U380291&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