L-Fucitol, pentakis(trifluoroacetate)

Inchi: InChI=1S/C16H9F15O10/c1-3(38-8(33)13(20,21)22)5(40-10(35)15(26,27)28)6(41-11(36)
InchiKey: NGTFCWJOYAUEKU-UHFFFAOYSA-N
Formula: C16H9F15O10
SMILES: CC(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)OC(=
Mol. weight [g/mol]: 646.21

Physical Properties

Property code	Value	Unit	Source
gf	-4003.47	kJ/mol	Joback Method
hf	-4604.09	kJ/mol	Joback Method
hfus	46.17	kJ/mol	Joback Method
hvap	76.70	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.008		Crippen Method
mcvol	300.050	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	1051.30		NIST Webbook
rinpol	1051.30		NIST Webbook
tb	918.07	K	Joback Method
tc	1135.26	K	Joback Method
tf	591.83	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.07	J/mol×K	918.07	Joback Method
cpg	989.26	J/mol×K	954.27	Joback Method
cpg	996.27	J/mol×K	990.47	Joback Method
cpg	1002.18	J/mol×K	1026.66	Joback Method
cpg	1007.07	J/mol×K	1062.86	Joback Method
cpg	1011.04	J/mol×K	1099.06	Joback Method
cpg	1014.16	J/mol×K	1135.26	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=U380211&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