D-Pinitol, pentakis(trifluoroacetate)

Inchi: InChI=1S/C17H9F15O11/c1-38-2-3(39-8(33)13(18,19)20)5(41-10(35)15(24,25)26)7(43-1
InchiKey: YUVUJOCAYPIZBU-UHFFFAOYSA-N
Formula: C17H9F15O11
SMILES: COC1C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1
Mol. weight [g/mol]: 674.22

Physical Properties

Property code	Value	Unit	Source
gf	-4104.39	kJ/mol	Joback Method
hf	-4783.21	kJ/mol	Joback Method
hfus	61.23	kJ/mol	Joback Method
hvap	81.78	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	2.385		Crippen Method
mcvol	309.150	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rinpol	1054.80		NIST Webbook
tb	961.33	K	Joback Method
tc	1190.26	K	Joback Method
tf	671.51	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.21	J/mol×K	961.33	Joback Method
cpg	1084.15	J/mol×K	999.48	Joback Method
cpg	1090.15	J/mol×K	1037.64	Joback Method
cpg	1094.27	J/mol×K	1075.79	Joback Method
cpg	1096.54	J/mol×K	1113.95	Joback Method
cpg	1097.01	J/mol×K	1152.10	Joback Method
cpg	1095.73	J/mol×K	1190.26	Joback Method

Sources

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=U380210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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