

N-Acetyl-D-galactosaminitol, pentakis(trifluoroacetate)

Inchi: InChI=1S/C18H12F15NO11/c1-4(35)34-5(2-41-9(36)14(19,20)21)7(44-12(39)17(28,29)3
InchiKey: QEIVUVSMPUBDA-UHFFFAOYSA-N
Formula: C18H12F15NO11
SMILES: CC(=O)NC(COC(=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)C(COC(=O)C(F)(F)F)
Mol. weight [g/mol]: 703.26

Physical Properties

Property code	Value	Unit	Source
gf	-4026.16	kJ/mol	Joback Method
hf	-4704.48	kJ/mol	Joback Method
hfus	58.05	kJ/mol	Joback Method
hvap	94.34	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	2.124		Crippen Method
mcvol	339.780	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpola	1394.30		NIST Webbook
rinpola	1394.30		NIST Webbook
tb	1067.87	K	Joback Method
tc	1359.21	K	Joback Method
tf	716.96	K	Joback Method
vc	1.395	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1138.97	J/molxK	1067.87	Joback Method
cpg	1145.17	J/molxK	1116.43	Joback Method
cpg	1149.68	J/molxK	1164.98	Joback Method
cpg	1152.71	J/molxK	1213.54	Joback Method
cpg	1154.50	J/molxK	1262.10	Joback Method
cpg	1155.26	J/molxK	1310.65	Joback Method
cpg	1155.21	J/molxK	1359.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380309&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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