Adonitol, pentakis(trifluoroacetate)

Inchi: InChI=1S/C15H7F15O10/c16-11(17,18)6(31)36-1-3(38-8(33)13(22,23)24)5(40-10(35)15(
InchiKey: VKRTZHFXBRDDBC-UHFFFAOYSA-N
Formula: C15H7F15O10
SMILES: O=C(OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)C
Mol. weight [g/mol]: 632.19

Physical Properties

Property code	Value	Unit	Source
gf	-4009.45	kJ/mol	Joback Method
hf	-4578.17	kJ/mol	Joback Method
hfus	47.10	kJ/mol	Joback Method
hvap	74.86	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.620		Crippen Method
mcvol	285.960	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	1039.20		NIST Webbook
rinpol	1039.20		NIST Webbook
tb	895.63	K	Joback Method
tc	1104.84	K	Joback Method
tf	595.56	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.57	J/mol×K	895.63	Joback Method
cpg	933.39	J/mol×K	930.50	Joback Method
cpg	940.12	J/mol×K	965.37	Joback Method
cpg	945.84	J/mol×K	1000.23	Joback Method
cpg	950.61	J/mol×K	1035.10	Joback Method
cpg	954.51	J/mol×K	1069.97	Joback Method
cpg	957.62	J/mol×K	1104.84	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=U380207&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

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