

D-(-)-Tagatopyranose, pentakis(trifluoroacetate) (isomer 2)

Inchi:	InChI=1S/C16H7F15O11/c17-12(18,19)6(32)37-2-11(42-10(36)16(29,30)31)5(41-9(35)1
InchiKey:	TVXVQZUZYLRUBY-UHFFFAOYSA-N
Formula:	C16H7F15O11
SMILES:	O=C(OCC1(OC(=O)C(F)(F)F)OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)
Mol. weight [g/mol]:	660.20

Physical Properties

Property code	Value	Unit	Source
gf	-4084.00	kJ/mol	Joback Method
hf	-4706.43	kJ/mol	Joback Method
hfus	56.99	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.346		Crippen Method
mcvol	295.060	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinsol	1182.50		NIST Webbook
tb	952.56	K	Joback Method
tc	1173.44	K	Joback Method
tf	696.96	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.67	J/molxK	952.56	Joback Method
cpg	1024.63	J/molxK	989.37	Joback Method
cpg	1035.04	J/molxK	1026.19	Joback Method
cpg	1045.07	J/molxK	1063.00	Joback Method
cpg	1054.87	J/molxK	1099.82	Joback Method
cpg	1064.59	J/molxK	1136.63	Joback Method
cpg	1074.39	J/molxK	1173.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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