

1-Chloro-1-deoxytagatose, tetrakis(trifluoroacetate), methyloxime

Inchi:	InChI=1S/C15H10ClF12NO9/c1-34-29-4(2-16)6(37-10(32)14(23,24)25)7(38-11(33)15(26
InchiKey:	FCKRVLAPGXEFND-UHFFFAOYSA-N
Formula:	C15H10ClF12NO9
SMILES:	CON=C(CCl)C(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
Mol. weight [g/mol]:	611.67

Physical Properties

Property code	Value	Unit	Source
hf	-3811.82	kJ/mol	Joback Method
hvap	79.64	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	2.755		Crippen Method
mcvol	297.000	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	1262.30		NIST Webbook
rinpol	1262.30		NIST Webbook
tb	961.17	K	Joback Method
tc	1182.36	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380287&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

hf:	Enthalpy of formation 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

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