

D-(+)-Glucuronic acid «gamma»-lactone, tris(trifluoroacetate) (isomer 1)

Inchi:	InChI=1S/C12H5F9O9/c13-10(14,15)7(23)28-3-1-2(26-5(3)22)4(29-8(24)11(16,17)18)6(2
InchiKey:	JTNJEXCWPOHXIX-UHFFFAOYSA-N
Formula:	C12H5F9O9
SMILES:	O=C1OC2C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)OC2C1OC(=O)C(F)(F)F
Mol. weight [g/mol]:	464.15

Physical Properties

Property code	Value	Unit	Source
hfus	51.43	kJ/mol	Joback Method
logp	0.690		Crippen Method
mcvol	209.780	ml/mol	McGowan Method
rinpol	1404.80		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.03	J/mol×K	816.30	Joback Method
cpg	717.68	J/mol×K	848.45	Joback Method
cpg	726.34	J/mol×K	880.60	Joback Method
cpg	734.02	J/mol×K	912.74	Joback Method
cpg	740.76	J/mol×K	944.89	Joback Method
cpg	746.59	J/mol×K	977.04	Joback Method
cpg	751.52	J/mol×K	1009.19	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U380254&Units=SI>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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