D-(+)-Glucuronic acid «gamma»-lactone, tris(trifluoroacetate) (isomer 2)

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	1428.20		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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U380255&Units=SI

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.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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

Latest version available from:
https://www.chemeo.com/cid/56-277-3/D-Glucuronic-acid-gamma-lactone-tris-trifluoroacetate-isomer-2.pdf
Generated by Cheméo on 2026-07-22 03:09:49.207463921 +0000 UTC m=+200885.049349301.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.