

4-O-ACETYL-2,5-DI-O-METHYL-3,6-DIDEOXY-D-G

Other names:	4-O-Acetyl-2,5-di-O-methyl-3,6-dideoxygluconitrile
Inchi:	InChI=1S/C10H17NO4/c1-7(13-3)10(15-8(2)12)5-9(6-11)14-4/h7,9-10H,5H2,1-4H3
InchiKey:	UIOZESJFWPMERW-UHFFFAOYSA-N
Formula:	C10H17NO4
SMILES:	COC(C#N)CC(OC(C)=O)C(C)OC
Mol. weight [g/mol]:	215.25

Physical Properties

Property code	Value	Unit	Source
hfus	17.76	kJ/mol	Joback Method
logp	0.882		Crippen Method
mcvol	172.320	ml/mol	McGowan Method
ripol	1335.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.04	J/mol×K	650.09	Joback Method
cpg	467.93	J/mol×K	682.75	Joback Method
cpg	480.19	J/mol×K	715.40	Joback Method
cpg	491.80	J/mol×K	748.06	Joback Method
cpg	502.74	J/mol×K	780.71	Joback Method
cpg	513.01	J/mol×K	813.37	Joback Method
cpg	522.58	J/mol×K	846.02	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U101803&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

Legend

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

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