Glucose, 2-methyl, nitrile, acetylated

Inchi: InChI=1S/C15H21NO9/c1-8(17)22-7-13(23-9(2)18)15(25-11(4)20)14(24-10(3)19)12(6-16
InchiKey: UNJPDBKOLFTASN-GBJTYRQASA-N
Formula: C15H21NO9
SMILES: COC(C#N)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 359.33

Physical Properties

Property code	Value	Unit	Source
gf	-841.84	kJ/mol	Joback Method
hf	-1320.59	kJ/mol	Joback Method
hfus	34.36	kJ/mol	Joback Method
hvap	96.94	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	-0.117		Crippen Method
mcvol	259.220	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	970.50	K	Joback Method
tc	1190.72	K	Joback Method
tf	574.67	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.47	J/mol×K	970.50	Joback Method
cpg	821.94	J/mol×K	1007.20	Joback Method
cpg	828.78	J/mol×K	1043.91	Joback Method
cpg	833.96	J/mol×K	1080.61	Joback Method
cpg	837.44	J/mol×K	1117.32	Joback Method
cpg	839.16	J/mol×K	1154.02	Joback Method
cpg	839.08	J/mol×K	1190.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530215&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

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

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