Glucose, 2,3,6-trimethyl, nitrile, acetylated

Inchi: InChI=1S/C13H21NO7/c1-8(15)20-11(7-17-3)13(21-9(2)16)12(19-5)10(6-14)18-4/h10-13
InchiKey: ZRJVYQQKDYYEET-UMSGYPCISA-N
Formula: C13H21NO7
SMILES: COCC(OC(C)=O)C(OC(C)=O)C(OC)C(C#N)OC
Mol. weight [g/mol]: 303.31

Physical Properties

Property code	Value	Unit	Source
gf	-600.84	kJ/mol	Joback Method
hf	-1054.15	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.050		Crippen Method
mcvol	227.900	ml/mol	McGowan Method
pc	1710.36	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1839.00		NIST Webbook
rinpol	1844.00		NIST Webbook
tb	817.00	K	Joback Method
tc	1017.55	K	Joback Method
tf	452.27	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.69	J/mol×K	817.00	Joback Method
cpg	696.28	J/mol×K	850.43	Joback Method
cpg	707.81	J/mol×K	883.85	Joback Method
cpg	718.26	J/mol×K	917.28	Joback Method
cpg	727.57	J/mol×K	950.70	Joback Method
cpg	735.73	J/mol×K	984.13	Joback Method
cpg	742.68	J/mol×K	1017.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R530097&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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