2-Deoxy-D-ribose, aldononitrile, triacetate

Inchi: InChI=1S/C11H15NO6/c1-7(13)16-6-11(18-9(3)15)10(4-5-12)17-8(2)14/h10-11H,4,6H2,1
InchiKey: QIPNLISJPJVKGP-UHFFFAOYSA-N
Formula: C11H15NO6
SMILES: CC(=O)OCC(OC(C)=O)C(CC#N)OC(C)=O
Mol. weight [g/mol]: 257.24

Physical Properties

Property code	Value	Unit	Source
gf	-531.72	kJ/mol	Joback Method
hf	-850.45	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.327		Crippen Method
mcvol	189.550	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1598.40		NIST Webbook
rinpol	1598.40		NIST Webbook
tb	781.15	K	Joback Method
tc	985.56	K	Joback Method
tf	465.20	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.09	J/mol×K	781.15	Joback Method
cpg	543.78	J/mol×K	815.22	Joback Method
cpg	553.65	J/mol×K	849.29	Joback Method
cpg	562.67	J/mol×K	883.36	Joback Method
cpg	570.84	J/mol×K	917.42	Joback Method
cpg	578.12	J/mol×K	951.49	Joback Method
cpg	584.51	J/mol×K	985.56	Joback Method

Sources

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=U380431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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