D-Allose, aldononitrile, pentaacetate

Inchi: InChI=1S/C16H21NO10/c1-8(18)23-7-14(25-10(3)20)16(27-12(5)22)15(26-11(4)21)13(6-
InchiKey: INCBLRCTSZYSJE-UHFFFAOYSA-N
Formula: C16H21NO10
SMILES: CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O
Mol. weight [g/mol]: 387.34

Physical Properties

Property code	Value	Unit	Source
gf	-962.34	kJ/mol	Joback Method
hf	-1453.81	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	-0.200		Crippen Method
mcvol	274.880	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	1909.40		NIST Webbook
tb	1047.25	K	Joback Method
tc	1282.15	K	Joback Method
tf	635.87	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.07	J/mol×K	1047.25	Joback Method
cpg	875.40	J/mol×K	1086.40	Joback Method
cpg	878.69	J/mol×K	1125.55	Joback Method
cpg	879.90	J/mol×K	1164.70	Joback Method
cpg	878.96	J/mol×K	1203.85	Joback Method
cpg	875.84	J/mol×K	1243.00	Joback Method
cpg	870.46	J/mol×K	1282.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380429&Units=SI

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