DL-Arabinose, aldononitrile, tetraacetate

Inchi: InChI=1S/C13H17NO8/c1-7(15)19-6-12(21-9(3)17)13(22-10(4)18)11(5-14)20-8(2)16/h11
InchiKey: YHTPKBYAZJOQCI-UHFFFAOYSA-N
Formula: C13H17NO8
SMILES: CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O
Mol. weight [g/mol]: 315.28

Physical Properties

Property code	Value	Unit	Source
gf	-751.24	kJ/mol	Joback Method
hf	-1141.81	kJ/mol	Joback Method
hfus	31.51	kJ/mol	Joback Method
hvap	90.47	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	-0.132		Crippen Method
mcvol	225.170	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1710.90		NIST Webbook
tb	902.76	K	Joback Method
tc	1116.10	K	Joback Method
tf	544.90	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.92	J/mol×K	902.76	Joback Method
cpg	685.12	J/mol×K	938.32	Joback Method
cpg	693.11	J/mol×K	973.87	Joback Method
cpg	699.85	J/mol×K	1009.43	Joback Method
cpg	705.31	J/mol×K	1044.99	Joback Method
cpg	709.46	J/mol×K	1080.55	Joback Method
cpg	712.26	J/mol×K	1116.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380421&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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