L-(-)-Fucose, aldononitrile, tetraacetate

Inchi: InChI=1S/C14H19NO8/c1-7(20-8(2)16)13(22-10(4)18)14(23-11(5)19)12(6-15)21-9(3)17/h
InchiKey: MMUJVSPMJDQIMU-UHFFFAOYSA-N
Formula: C14H19NO8
SMILES: CC(=O)OC(C)C(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O
Mol. weight [g/mol]: 329.30

Physical Properties

Property code	Value	Unit	Source
gf	-745.26	kJ/mol	Joback Method
hf	-1167.73	kJ/mol	Joback Method
hfus	30.58	kJ/mol	Joback Method
hvap	92.31	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	0.257		Crippen Method
mcvol	239.260	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	1720.40		NIST Webbook
rinpol	1720.40		NIST Webbook
tb	925.20	K	Joback Method
tc	1141.12	K	Joback Method
tf	541.17	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.37	J/mol×K	925.20	Joback Method
cpg	741.72	J/mol×K	961.19	Joback Method
cpg	749.74	J/mol×K	997.17	Joback Method
cpg	756.40	J/mol×K	1033.16	Joback Method
cpg	761.67	J/mol×K	1069.14	Joback Method
cpg	765.52	J/mol×K	1105.13	Joback Method
cpg	767.92	J/mol×K	1141.12	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=U380432&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