L-(+)-Threose, aldononitrile, triacetate

Inchi: InChI=1S/C10H13NO6/c1-6(12)15-5-10(17-8(3)14)9(4-11)16-7(2)13/h9-10H,5H2,1-3H3
InchiKey: ZLZTVHJXGGNLSP-UHFFFAOYSA-N
Formula: C10H13NO6
SMILES: CC(=O)OCC(OC(C)=O)C(C#N)OC(C)=O
Mol. weight [g/mol]: 243.21

Physical Properties

Property code	Value	Unit	Source
gf	-540.14	kJ/mol	Joback Method
hf	-829.81	kJ/mol	Joback Method
hfus	24.48	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	-0.064		Crippen Method
mcvol	175.460	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1454.40		NIST Webbook
tb	758.27	K	Joback Method
tc	964.28	K	Joback Method
tf	453.93	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.42	J/mol×K	758.27	Joback Method
cpg	490.64	J/mol×K	792.61	Joback Method
cpg	500.09	J/mol×K	826.94	Joback Method
cpg	508.76	J/mol×K	861.28	Joback Method
cpg	516.62	J/mol×K	895.61	Joback Method
cpg	523.66	J/mol×K	929.95	Joback Method
cpg	529.84	J/mol×K	964.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380425&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

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