L-xylo-hexulosonic acid, methyl ester

Other names: L-xylo-2-Hexulosonic acid, methyl ester
Inchi: InChI=1S/C7H12O7/c1-14-7(13)6(12)5(11)4(10)3(9)2-8/h3-5,8-11H,2H2,1H3
InchiKey: KPHIBLNUVRGOGU-UHFFFAOYSA-N
Formula: C7H12O7
SMILES: COC(=O)C(=O)C(O)C(O)C(O)CO
Mol. weight [g/mol]: 208.17
CAS: 3031-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-909.38	kJ/mol	Joback Method
hf	-1169.95	kJ/mol	Joback Method
hfus	24.06	kJ/mol	Joback Method
hvap	112.63	kJ/mol	Joback Method
log10ws	1.71		Crippen Method
logp	-3.197		Crippen Method
mcvol	141.980	ml/mol	McGowan Method
pc	5183.17	kPa	Joback Method
tb	857.12	K	Joback Method
tc	1049.51	K	Joback Method
tf	489.02	K	Joback Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.30	J/mol×K	857.12	Joback Method
cpg	455.58	J/mol×K	1017.45	Joback Method
cpg	451.29	J/mol×K	985.38	Joback Method
cpg	446.52	J/mol×K	953.32	Joback Method
cpg	441.27	J/mol×K	921.25	Joback Method
cpg	435.54	J/mol×K	889.19	Joback Method
cpg	459.40	J/mol×K	1049.51	Joback Method
dvisc	0.0000002	Pa×s	857.12	Joback Method

dvisc	0.0000004	Pa×s	795.77	Joback Method
dvisc	0.0000010	Pa×s	734.42	Joback Method
dvisc	0.0000028	Pa×s	673.07	Joback Method
dvisc	0.0000100	Pa×s	611.72	Joback Method
dvisc	0.0000476	Pa×s	550.37	Joback Method
dvisc	0.0003362	Pa×s	489.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3031989&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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume