Laminaritriose, permethyl

Inchi: InChI=1S/C27H50O16/c1-28-12-13-14(29-2)15(30-3)18(31-4)26(39-13)40-17-21(34-7)25
InchiKey: GIDNCUSCVDMDSU-OBPAOPMPSA-N
Formula: C27H50O16
SMILES: COCC1OC(OC2C(OC)C(OC)OC(OC3C(OC)C(OC)OC(OC)C3OC)C2OC)C(OC)C(OC)C
Mol. weight [g/mol]: 630.68

Physical Properties

Property code	Value	Unit	Source
gf	-1466.07	kJ/mol	Joback Method
hf	-2796.59	kJ/mol	Joback Method
hfus	93.42	kJ/mol	Joback Method
hvap	118.14	kJ/mol	Joback Method
log10ws	-0.36		Crippen Method
logp	-0.463		Crippen Method
mcvol	452.630	ml/mol	McGowan Method
pc	678.52	kPa	Joback Method
rinpol	3171.00		NIST Webbook
rinpol	3171.00		NIST Webbook
tb	1192.08	K	Joback Method
tc	1486.66	K	Joback Method
tf	734.01	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1771.81	J/mol×K	1192.08	Joback Method
cpg	1753.75	J/mol×K	1241.18	Joback Method
cpg	1724.66	J/mol×K	1290.27	Joback Method
cpg	1684.03	J/mol×K	1339.37	Joback Method
cpg	1631.32	J/mol×K	1388.47	Joback Method
cpg	1566.02	J/mol×K	1437.57	Joback Method
cpg	1487.60	J/mol×K	1486.66	Joback Method
dvisc	0.0000719	Pa×s	734.01	Joback Method

dvisc	0.0000520	Pa×s	810.36	Joback Method
dvisc	0.0000398	Pa×s	886.70	Joback Method
dvisc	0.0000318	Pa×s	963.04	Joback Method
dvisc	0.0000262	Pa×s	1039.39	Joback Method
dvisc	0.0000222	Pa×s	1115.73	Joback Method
dvisc	0.0000192	Pa×s	1192.08	Joback Method

Sources

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=R151169&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume