Laminaritetraose, permethyl

Inchi: InChI=1S/C35H64O21/c1-36-15-16-17(37-2)18(38-3)22(39-4)33(50-16)51-20-25(42-7)31
InchiKey: INQZLNRGEBCQQW-YOADXIJLSA-N
Formula: C35H64O21
SMILES: COCC1OC(OC2C(OC)C(OC)OC(OC3C(OC)C(OC)OC(OC4C(OC)C(OC)OC(OC)C4OC)
Mol. weight [g/mol]: 820.87

Physical Properties

Property code	Value	Unit	Source
gf	-1911.22	kJ/mol	Joback Method
hf	-3649.63	kJ/mol	Joback Method
hfus	122.99	kJ/mol	Joback Method
hvap	149.29	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	-0.719		Crippen Method
mcvol	583.840	ml/mol	McGowan Method
pc	470.34	kPa	Joback Method
rinpol	4049.00		NIST Webbook
tb	1492.62	K	Joback Method
tc	2058.11	K	Joback Method
tf	930.08	K	Joback Method
vc	2.102	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1903.42	J/mol×K	1492.62	Joback Method
cpg	1649.16	J/mol×K	1586.87	Joback Method
cpg	1323.63	J/mol×K	1681.12	Joback Method
cpg	921.94	J/mol×K	1775.36	Joback Method
cpg	439.20	J/mol×K	1869.61	Joback Method
cpg	-129.48	J/mol×K	1963.86	Joback Method
cpg	-788.99	J/mol×K	2058.11	Joback Method
dvisc	0.0000214	Pa×s	930.08	Joback Method
dvisc	0.0000157	Pa×s	1023.84	Joback Method

dvisc	0.0000122	Pa×s	1117.59	Joback Method
dvisc	0.0000098	Pa×s	1211.35	Joback Method
dvisc	0.0000081	Pa×s	1305.11	Joback Method
dvisc	0.0000069	Pa×s	1398.86	Joback Method
dvisc	0.0000060	Pa×s	1492.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R151154&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume