Isomaltotetraose, permethyl

Inchi: InChI=1S/C37H68O21/c1-39-16-19-23(43-5)29(47-9)34(51-13)57-33(19)55-26(21(42-4)1
InchiKey: IHGBCBCBAWXHHN-QUOYLCKYSA-N
Formula: C37H68O21
SMILES: COCC(OC)C(OC1OC(OC)C(OC)C(OC)C1COC)C(OC1OC(COC)C(OC)C(OC)C1OC)C(O
Mol. weight [g/mol]: 848.92

Physical Properties

Property code	Value	Unit	Source
gf	-1911.15	kJ/mol	Joback Method
hf	-3638.57	kJ/mol	Joback Method
hfus	112.27	kJ/mol	Joback Method
hvap	155.20	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.586		Crippen Method
mcvol	618.580	ml/mol	McGowan Method
pc	441.17	kPa	Joback Method
rinpol	4017.00		NIST Webbook
tb	1557.46	K	Joback Method
tc	2298.49	K	Joback Method
tf	917.63	K	Joback Method
vc	2.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1880.27	J/mol×K	1557.46	Joback Method
cpg	1510.45	J/mol×K	1680.96	Joback Method
cpg	1021.91	J/mol×K	1804.47	Joback Method
cpg	405.11	J/mol×K	1927.97	Joback Method
cpg	-349.46	J/mol×K	2051.48	Joback Method
cpg	-1251.32	J/mol×K	2174.98	Joback Method
cpg	-2309.99	J/mol×K	2298.49	Joback Method
dvisc	0.0000058	Pa×s	917.63	Joback Method
dvisc	0.0000035	Pa×s	1024.27	Joback Method

dvisc	0.0000024	Pa×s	1130.91	Joback Method
dvisc	0.0000017	Pa×s	1237.55	Joback Method
dvisc	0.0000013	Pa×s	1344.18	Joback Method
dvisc	0.0000010	Pa×s	1450.82	Joback Method
dvisc	0.0000008	Pa×s	1557.46	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=R151109&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
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