Maltotriose, permethyl

Inchi: InChI=1S/C29H54O16/c1-30-12-15-18(33-4)21(34-5)25(38-9)28(42-15)45-20-17(14-32-3
InchiKey: LNAZSHAWQACDHT-UHFFFAOYSA-N
Formula: C29H54O16
SMILES: COCC1OC(OC2C(COC)OC(OC3C(COC)OC(OC)C(OC)C3OC)C(OC)C2OC)C(OC)C(OC
Mol. weight [g/mol]: 658.73

Physical Properties

Property code	Value	Unit	Source
gf	-1449.23	kJ/mol	Joback Method
hf	-2837.87	kJ/mol	Joback Method
hfus	98.60	kJ/mol	Joback Method
hvap	122.59	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	-0.378		Crippen Method
mcvol	480.810	ml/mol	McGowan Method
pc	615.42	kPa	Joback Method
rinpol	3095.00		NIST Webbook
rinpol	3095.00		NIST Webbook
tb	1237.84	K	Joback Method
tc	1564.56	K	Joback Method
tf	756.55	K	Joback Method
vc	1.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1867.12	J/mol×K	1237.84	Joback Method
cpg	1836.61	J/mol×K	1292.29	Joback Method
cpg	1791.76	J/mol×K	1346.75	Joback Method
cpg	1731.89	J/mol×K	1401.20	Joback Method
cpg	1656.31	J/mol×K	1455.65	Joback Method
cpg	1564.33	J/mol×K	1510.11	Joback Method
cpg	1455.25	J/mol×K	1564.56	Joback Method
dvisc	0.0000584	Pa×s	756.55	Joback Method

dvisc	0.0000414	Pa×s	836.77	Joback Method
dvisc	0.0000312	Pa×s	916.98	Joback Method
dvisc	0.0000246	Pa×s	997.20	Joback Method
dvisc	0.0000201	Pa×s	1077.41	Joback Method
dvisc	0.0000169	Pa×s	1157.63	Joback Method
dvisc	0.0000145	Pa×s	1237.84	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U394591&Units=SI

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