

Stachyose, permethyl

Inchi:	InChI=1S/C38H70O21/c1-39-15-20-24(42-4)28(46-8)31(49-11)35(55-20)53-17-21-25(43-41)29-37-33-35-31-29-25-21-17-15-11-7-3
InchiKey:	UAFWRHUGEGBPTGM-NYOZWESTSA-N
Formula:	C38H70O21
SMILES:	COCC1OC(OCC2OC(OCC3OC(OC4(COC)OC(COC)C(OC)C4OC)C(OC)C(OC)C3OC)OC)OC
Mol. weight [g/mol]:	862.95

Physical Properties

Property code	Value	Unit	Source
gf	-1871.64	kJ/mol	Joback Method
hf	-3669.81	kJ/mol	Joback Method
hfus	125.50	kJ/mol	Joback Method
hvap	154.95	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	-0.590		Crippen Method
mcvol	626.110	ml/mol	McGowan Method
pc	425.83	kPa	Joback Method
rinpol	3873.00		NIST Webbook
tb	1561.90	K	Joback Method
tc	2268.09	K	Joback Method
tf	995.55	K	Joback Method
vc	2.276	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2174.27	J/molxK	1561.90	Joback Method
cpg	1911.89	J/molxK	1679.60	Joback Method
cpg	1563.45	J/molxK	1797.30	Joback Method
cpg	1123.28	J/molxK	1914.99	Joback Method
cpg	585.66	J/molxK	2032.69	Joback Method
cpg	-55.09	J/molxK	2150.39	Joback Method
cpg	-804.67	J/molxK	2268.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R151243&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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