Sophorose, permethyl

Inchi: InChI=1S/C20H38O11/c1-21-9-11-14(24-4)16(26-6)18(19(28-8)29-11)31-20-17(27-7)15(
InchiKey: JIBCAZMNXQQBIE-JOVUISTQSA-N
Formula: C20H38O11
SMILES: COCC1OC(OC2C(OC)OC(COC)C(OC)C2OC)C(OC)C(OC)C1OC
Mol. weight [g/mol]: 454.51

Physical Properties

Property code	Value	Unit	Source
gf	-1012.50	kJ/mol	Joback Method
hf	-1964.19	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	-0.164		Crippen Method
mcvol	335.510	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	2329.00		NIST Webbook
tb	914.42	K	Joback Method
tc	1121.61	K	Joback Method
tf	549.21	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.05	J/mol×K	914.42	Joback Method
cpg	1257.67	J/mol×K	948.95	Joback Method
cpg	1273.53	J/mol×K	983.48	Joback Method
cpg	1286.53	J/mol×K	1018.01	Joback Method
cpg	1296.53	J/mol×K	1052.54	Joback Method
cpg	1303.43	J/mol×K	1087.07	Joback Method
cpg	1307.10	J/mol×K	1121.61	Joback Method
dvisc	0.0002167	Pa×s	549.21	Joback Method
dvisc	0.0001503	Pa×s	610.08	Joback Method

dvisc	0.0001114	Pa×s	670.95	Joback Method
dvisc	0.0000868	Pa×s	731.82	Joback Method
dvisc	0.0000703	Pa×s	792.68	Joback Method
dvisc	0.0000586	Pa×s	853.55	Joback Method
dvisc	0.0000501	Pa×s	914.42	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=R151238&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

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