Melezitose, monohydrate

Inchi: InChI=1S/C18H32O16/c19-1-5-8(23)11(26)13(28)16(30-5)32-15-10(25)7(3-21)33-18(15,
InchiKey: QWIZNVHXZXRPDR-UHFFFAOYSA-N
Formula: C18H32O16
SMILES: OCC1OC(OC2C(O)C(CO)OC2(CO)OC2OC(CO)C(O)C(O)C2O)C(O)C(O)C1O
Mol. weight [g/mol]: 504.44

Physical Properties

Property code	Value	Unit	Source
gf	-1877.55	kJ/mol	Joback Method
hf	-2789.20	kJ/mol	Joback Method
hfus	96.75	kJ/mol	Joback Method
hvap	254.05	kJ/mol	Joback Method
log10ws	2.57		Crippen Method
logp	-7.571		Crippen Method
mcvol	325.820	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	1754.16	K	Joback Method
tc	4228.42	K	Joback Method
tf	1088.73	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1440.80	J/mol×K	1754.16	Joback Method
cpg	1455.79	J/mol×K	2166.54	Joback Method
cpg	1539.35	J/mol×K	2578.91	Joback Method
cpg	1784.73	J/mol×K	2991.29	Joback Method
cpg	2285.15	J/mol×K	3403.66	Joback Method
cpg	3133.87	J/mol×K	3816.04	Joback Method
cpg	4424.11	J/mol×K	4228.42	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=B6007575&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume