

Sucrose monopalmitate

Inchi:	InChI=1S/C28H52O12/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21(31)37-17-20-22(32)24(33)25(34)26(35)27(36)38
InchiKey:	XYFGTTCGHCGTDZ-UHFFFAOYSA-N
Formula:	C28H52O12
SMILES:	CCCCCCCCCCCCCCCC(=O)OCC1OC(OC2(CO)OC(CO)C(O)C2O)C(O)C(O)C1O
Mol. weight [g/mol]:	580.71
CAS:	13039-41-3

Physical Properties

Property code	Value	Unit	Source
gf	-1282.48	kJ/mol	Joback Method
hf	-2340.22	kJ/mol	Joback Method
hfus	103.79	kJ/mol	Joback Method
hvap	212.63	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	0.637		Crippen Method
mcvol	449.800	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
tb	1640.29	K	Joback Method
tc	3293.54	K	Joback Method
tf	991.09	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2009.99	J/molxK	1640.29	Joback Method
cpg	2162.50	J/molxK	1915.83	Joback Method
cpg	2394.97	J/molxK	2191.37	Joback Method
cpg	2758.14	J/molxK	2466.91	Joback Method
cpg	3302.76	J/molxK	2742.45	Joback Method
cpg	4079.56	J/molxK	3018.00	Joback Method
cpg	5139.30	J/molxK	3293.54	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=C13039413&Units=SI

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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