

Sucrose dipalmitate

Inchi:

InChI=1S/C44H82O13/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-36(46)53-32-35-38(48

InchiKey:

HQQGQPZMCTVNNX-UHFFFAOYSA-N

Formula:

C44H82O13

SMILES:

CCCCCCCCCCCCCCCC(=O)OCC1OC(OC2(COC(=O)CCCCCCCCCCCCCCCC)OC(CO

Mol. weight [g/mol]:

819.11

CAS:

248917-86-4

Physical Properties

Property code	Value	Unit	Source
gf	-1244.86	kJ/mol	Joback Method
hf	-2763.03	kJ/mol	Joback Method
hfus	143.93	kJ/mol	Joback Method
hvap	240.73	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	6.669		Crippen Method
mcvol	676.810	ml/mol	McGowan Method
pc	465.68	kPa	Joback Method
tb	1990.48	K	Joback Method
tc	14441.53	K	Joback Method
tf	1182.75	K	Joback Method
vc	2.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3111.43	J/mol×K	1990.48	Joback Method
cpg	11838.42	J/mol×K	4065.66	Joback Method
cpg	53704.20	J/mol×K	6140.83	Joback Method
cpg	156645.15	J/mol×K	8216.01	Joback Method
cpg	348597.63	J/mol×K	10291.18	Joback Method
cpg	657498.04	J/mol×K	12366.36	Joback Method
cpg	1111282.74	J/mol×K	14441.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C248917864&Units=SI
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

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

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