

Sorbitan, tristearate

Inchi:	InChI=1S/C60H114O8/c1-4-7-10-13-16-19-22-25-28-31-34-37-40-43-46-49-56(61)65-53
InchiKey:	NBIZFEQHL SJRPG-UHFFFAOYSA-N
Formula:	C60H114O8
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCC(OC(=O)CCCCCCCCCCCCCCCCCCC)C1OCC(OC(=O)CCCCCCCCCCCCCCCCCCC)C1
Mol. weight [g/mol]:	963.54
CAS:	26658-19-5

Physical Properties

Property code	Value	Unit	Source
gf	-451.69	kJ/mol	Joback Method
hf	-2285.84	kJ/mol	Joback Method
hfus	164.14	kJ/mol	Joback Method
hvap	197.06	kJ/mol	Joback Method
log10ws	-20.22		Crippen Method
logp	17.897		Crippen Method
mvol	879.460	ml/mol	McGowan Method
pc	227.15	kPa	Joback Method
tb	1925.70	K	Joback Method
tc	10622.89	K	Joback Method
tf	1057.25	K	Joback Method
vc	3.441	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3526.22	J/molxK	1925.70	Joback Method
cpg	190013.24	J/molxK	9173.36	Joback Method
cpg	98678.29	J/molxK	7723.82	Joback Method
cpg	43407.38	J/molxK	6274.29	Joback Method
cpg	15155.25	J/molxK	4824.76	Joback Method
cpg	4876.62	J/molxK	3375.23	Joback Method
cpg	326457.49	J/molxK	10622.89	Joback Method
dvisc	6.0711175e-09	Paxs	1925.70	Joback Method
dvisc	8.6779389e-09	Paxs	1780.96	Joback Method

dvisc	1.3213373e-08	Paxs	1636.22	Joback Method
dvisc	2.1829883e-08	Paxs	1491.47	Joback Method
dvisc	4.0175086e-08	Paxs	1346.73	Joback Method
dvisc	8.5636931e-08	Paxs	1201.99	Joback Method
dvisc	0.0000002	Paxs	1057.25	Joback Method

Sources

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=C26658195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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