

Sebacic acid, 3,5-dimethylphenyl dodecyl ester

Inchi:	InChI=1S/C30H50O4/c1-4-5-6-7-8-9-10-13-16-19-22-33-29(31)20-17-14-11-12-15-18-21
InchiKey:	LKDILIQZGRIQRF-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	-172.97	kJ/mol	Joback Method
hf	-938.54	kJ/mol	Joback Method
hfus	72.29	kJ/mol	Joback Method
hvap	104.29	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.794		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	728.49	kPa	Joback Method
rinpol	3574.00		NIST Webbook
tb	1075.02	K	Joback Method
tc	1331.15	K	Joback Method
tf	623.64	K	Joback Method
vc	1.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.08	J/molxK	1075.02	Joback Method
cpg	1569.31	J/molxK	1288.46	Joback Method
cpg	1558.64	J/molxK	1245.77	Joback Method
cpg	1546.08	J/molxK	1203.08	Joback Method
cpg	1531.53	J/molxK	1160.40	Joback Method
cpg	1514.89	J/molxK	1117.71	Joback Method
cpg	1578.16	J/molxK	1331.15	Joback Method
dvisc	0.0000126	Paxs	1075.02	Joback Method
dvisc	0.0000164	Paxs	999.79	Joback Method

dvisc	0.0000224	Paxs	924.56	Joback Method
dvisc	0.0000323	Paxs	849.33	Joback Method
dvisc	0.0000498	Paxs	774.10	Joback Method
dvisc	0.0000846	Paxs	698.87	Joback Method
dvisc	0.0001630	Paxs	623.64	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=U354600&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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