

Sebacic acid, 3,5-dimethylphenyl undecyl ester

Inchi:	InChI=1S/C29H48O4/c1-4-5-6-7-8-9-12-15-18-21-32-28(30)19-16-13-10-11-14-17-20-29
InchiKey:	AXZWVNZRESMDOK-UHFFFAOYSA-N
Formula:	C29H48O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	460.69

Physical Properties

Property code	Value	Unit	Source
gf	-181.39	kJ/mol	Joback Method
hf	-917.90	kJ/mol	Joback Method
hfus	69.70	kJ/mol	Joback Method
hvap	102.06	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.404		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	767.76	kPa	Joback Method
rinpol	3460.00		NIST Webbook
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tb	1052.14	K	Joback Method
tc	1297.56	K	Joback Method
tf	612.37	K	Joback Method
vc	1.599	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.39	J/molxK	1052.14	Joback Method
cpg	1450.82	J/molxK	1093.04	Joback Method
cpg	1467.25	J/molxK	1133.95	Joback Method
cpg	1481.77	J/molxK	1174.85	Joback Method
cpg	1494.45	J/molxK	1215.75	Joback Method
cpg	1505.36	J/molxK	1256.65	Joback Method
cpg	1514.58	J/molxK	1297.56	Joback Method
dvisc	0.0001852	Paxs	612.37	Joback Method

dvisc	0.0000969	Paxs	685.66	Joback Method
dvisc	0.0000575	Paxs	758.96	Joback Method
dvisc	0.0000374	Paxs	832.25	Joback Method
dvisc	0.0000261	Paxs	905.55	Joback Method
dvisc	0.0000192	Paxs	978.84	Joback Method
dvisc	0.0000147	Paxs	1052.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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