Sebacic acid, 3,4-dimethylphenyl undecyl ester

Inchi: InChI=1S/C29H48O4/c1-4-5-6-7-8-9-12-15-18-23-32-28(30)19-16-13-10-11-14-17-20-29

InchiKey: GFSWGIWIDFHJQW-UHFFFAOYSA-N

Formula: C29H48O4

SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(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
mcvol	410.590	ml/mol	McGowan Method
pc	767.76	kPa	Joback Method
rinpol	3537.00		NIST Webbook
rinpol	3537.00		NIST Webbook
tb	1052.14	K	Joback Method
tc	1297.56	K	Joback Method
tf	612.37	K	Joback Method
vc	1.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1432.39	J/mol×K	1052.14	Joback Method
cpg	1505.36	J/mol×K	1256.65	Joback Method
cpg	1494.45	J/mol×K	1215.75	Joback Method
cpg	1481.77	J/mol×K	1174.85	Joback Method
cpg	1467.25	J/mol×K	1133.95	Joback Method
cpg	1450.82	J/mol×K	1093.04	Joback Method
cpg	1514.58	J/mol×K	1297.56	Joback Method
dvisc	0.0000147	Pa×s	1052.14	Joback Method

dvisc	0.0000192	Pa×s	978.84	Joback Method
dvisc	0.0000261	Pa×s	905.55	Joback Method
dvisc	0.0000374	Pa×s	832.25	Joback Method
dvisc	0.0000575	Pa×s	758.96	Joback Method
dvisc	0.0000969	Pa×s	685.66	Joback Method
dvisc	0.0001852	Pa×s	612.37	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=U354586&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