Sebacic acid, 2,5-dimethylphenyl dodecyl ester

Inchi: InChI=1S/C30H50O4/c1-4-5-6-7-8-9-10-13-16-19-24-33-29(31)20-17-14-11-12-15-18-21

InchiKey: MVQSVTRVDIDLLI-UHFFFAOYSA-N

Formula: C30H50O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)ccc1C

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	3503.00		NIST Webbook
tb	1075.02	K	Joback Method
tc	1331.15	K	Joback Method
tf	623.64	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.08	J/mol×K	1075.02	Joback Method
cpg	1514.89	J/mol×K	1117.71	Joback Method
cpg	1531.53	J/mol×K	1160.40	Joback Method
cpg	1546.08	J/mol×K	1203.08	Joback Method
cpg	1558.64	J/mol×K	1245.77	Joback Method
cpg	1569.31	J/mol×K	1288.46	Joback Method
cpg	1578.16	J/mol×K	1331.15	Joback Method
dvisc	0.0001630	Pa×s	623.64	Joback Method
dvisc	0.0000846	Pa×s	698.87	Joback Method

dvisc	0.0000498	Pa×s	774.10	Joback Method
dvisc	0.0000323	Pa×s	849.33	Joback Method
dvisc	0.0000224	Pa×s	924.56	Joback Method
dvisc	0.0000164	Pa×s	999.79	Joback Method
dvisc	0.0000126	Pa×s	1075.02	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=U354983&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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