Sebacic acid, dodecyl 3-propylphenyl ester

Inchi: InChI=1S/C31H52O4/c1-3-5-6-7-8-9-10-13-16-21-27-34-30(32)25-17-14-11-12-15-18-26
InchiKey: CXFUTFFGSPSMCD-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1CCC
Mol. weight [g/mol]: 488.74

Physical Properties

Property code	Value	Unit	Source
gf	-154.92	kJ/mol	Joback Method
hf	-947.71	kJ/mol	Joback Method
hfus	75.27	kJ/mol	Joback Method
hvap	105.85	kJ/mol	Joback Method
log10ws	-10.24		Crippen Method
logp	9.129		Crippen Method
mcvol	438.770	ml/mol	McGowan Method
pc	697.65	kPa	Joback Method
rinpol	3549.00		NIST Webbook
tb	1092.92	K	Joback Method
tc	1359.52	K	Joback Method
tf	622.39	K	Joback Method
vc	1.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1560.85	J/mol×K	1092.92	Joback Method
cpg	1580.35	J/mol×K	1137.35	Joback Method
cpg	1597.56	J/mol×K	1181.79	Joback Method
cpg	1612.60	J/mol×K	1226.22	Joback Method
cpg	1625.59	J/mol×K	1270.65	Joback Method
cpg	1636.65	J/mol×K	1315.09	Joback Method
cpg	1645.91	J/mol×K	1359.52	Joback Method
dvisc	0.0001601	Pa×s	622.39	Joback Method
dvisc	0.0000787	Pa×s	700.81	Joback Method

dvisc	0.0000447	Pa×s	779.23	Joback Method
dvisc	0.0000281	Pa×s	857.66	Joback Method
dvisc	0.0000191	Pa×s	936.08	Joback Method
dvisc	0.0000138	Pa×s	1014.50	Joback Method
dvisc	0.0000104	Pa×s	1092.92	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U355060&Units=SI

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