Adipic acid, hexadecyl 2-propylphenyl ester

Inchi: InChI=1S/C31H52O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-21-27-34-30(32)25-19-20-26
InchiKey: POIIOYBDXVFVAQ-UHFFFAOYSA-N
Formula: C31H52O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=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	3482.00		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	1636.65	J/mol×K	1315.09	Joback Method
cpg	1625.59	J/mol×K	1270.65	Joback Method
cpg	1612.60	J/mol×K	1226.22	Joback Method
cpg	1597.56	J/mol×K	1181.79	Joback Method
cpg	1580.35	J/mol×K	1137.35	Joback Method
cpg	1645.91	J/mol×K	1359.52	Joback Method
dvisc	0.0000104	Pa×s	1092.92	Joback Method
dvisc	0.0000138	Pa×s	1014.50	Joback Method

dvisc	0.0000191	Pa×s	936.08	Joback Method
dvisc	0.0000281	Pa×s	857.66	Joback Method
dvisc	0.0000447	Pa×s	779.23	Joback Method
dvisc	0.0000787	Pa×s	700.81	Joback Method
dvisc	0.0001601	Pa×s	622.39	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=U353839&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