Sebacic acid, octyl 2-phenylphenyl ester

Inchi: InChI=1S/C30H42O4/c1-2-3-4-5-10-18-25-33-29(31)23-14-8-6-7-9-15-24-30(32)34-28-22
InchiKey: RCMVDPKDZPTNSI-UHFFFAOYSA-N
Formula: C30H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 466.65

Physical Properties

Property code	Value	Unit	Source
gf	-50.93	kJ/mol	Joback Method
hf	-690.54	kJ/mol	Joback Method
hfus	66.72	kJ/mol	Joback Method
hvap	105.90	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	8.284		Crippen Method
mcvol	400.920	ml/mol	McGowan Method
pc	886.30	kPa	Joback Method
rinpol	3495.00		NIST Webbook
tb	1096.72	K	Joback Method
tc	1345.52	K	Joback Method
tf	637.54	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1384.72	J/mol×K	1096.72	Joback Method
cpg	1443.90	J/mol×K	1304.05	Joback Method
cpg	1435.15	J/mol×K	1262.58	Joback Method
cpg	1424.97	J/mol×K	1221.12	Joback Method
cpg	1413.23	J/mol×K	1179.65	Joback Method
cpg	1399.85	J/mol×K	1138.19	Joback Method
cpg	1451.30	J/mol×K	1345.52	Joback Method
dvisc	0.0000128	Pa×s	1096.72	Joback Method
dvisc	0.0000166	Pa×s	1020.19	Joback Method

dvisc	0.0000227	Pa×s	943.66	Joback Method
dvisc	0.0000326	Pa×s	867.13	Joback Method
dvisc	0.0000503	Pa×s	790.60	Joback Method
dvisc	0.0000852	Pa×s	714.07	Joback Method
dvisc	0.0001638	Pa×s	637.54	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=U355069&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