Sebacic acid, decyl 1-phenylpropyl ester

Inchi: InChI=1S/C29H48O4/c1-3-5-6-7-8-11-14-20-25-32-28(30)23-18-12-9-10-13-19-24-29(31)
InchiKey: YRHHYNFUZCCWDE-UHFFFAOYSA-N
Formula: C29H48O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 460.69

Physical Properties

Property code	Value	Unit	Source
gf	-164.57	kJ/mol	Joback Method
hf	-900.24	kJ/mol	Joback Method
hfus	66.96	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.486		Crippen Method
mcvol	410.590	ml/mol	McGowan Method
pc	784.19	kPa	Joback Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook
tb	1041.74	K	Joback Method
tc	1282.47	K	Joback Method
tf	572.33	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.95	J/mol×K	1041.74	Joback Method
cpg	1509.25	J/mol×K	1242.35	Joback Method
cpg	1497.56	J/mol×K	1202.23	Joback Method
cpg	1484.27	J/mol×K	1162.11	Joback Method
cpg	1469.30	J/mol×K	1121.98	Joback Method
cpg	1452.55	J/mol×K	1081.86	Joback Method
cpg	1519.45	J/mol×K	1282.47	Joback Method
dvisc	0.0000127	Pa×s	1041.74	Joback Method

dvisc	0.0000171	Pa×s	963.50	Joback Method
dvisc	0.0000243	Pa×s	885.27	Joback Method
dvisc	0.0000371	Pa×s	807.03	Joback Method
dvisc	0.0000618	Pa×s	728.80	Joback Method
dvisc	0.0001167	Pa×s	650.56	Joback Method
dvisc	0.0002620	Pa×s	572.33	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=U354993&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