Sebacic acid, decyl 3-phenylallyl ester

Inchi: InChI=1S/C29H46O4/c1-2-3-4-5-6-9-12-18-25-32-28(30)23-16-10-7-8-11-17-24-29(31)33
InchiKey: AGHOMVBRWVWVJI-ZBJSNUHESA-N
Formula: C29H46O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-81.91	kJ/mol	Joback Method
hf	-777.74	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	100.69	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.048		Crippen Method
mcvol	406.290	ml/mol	McGowan Method
pc	803.88	kPa	Joback Method
rinpol	3535.00		NIST Webbook
tb	1046.34	K	Joback Method
tc	1287.17	K	Joback Method
tf	582.25	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1405.04	J/mol×K	1046.34	Joback Method
cpg	1483.13	J/mol×K	1247.03	Joback Method
cpg	1470.30	J/mol×K	1206.89	Joback Method
cpg	1456.18	J/mol×K	1166.75	Joback Method
cpg	1440.67	J/mol×K	1126.62	Joback Method
cpg	1423.66	J/mol×K	1086.48	Joback Method
cpg	1494.78	J/mol×K	1287.17	Joback Method
dvisc	0.0000123	Pa×s	1046.34	Joback Method
dvisc	0.0000164	Pa×s	968.99	Joback Method

dvisc	0.0000230	Pa×s	891.64	Joback Method
dvisc	0.0000344	Pa×s	814.29	Joback Method
dvisc	0.0000560	Pa×s	736.95	Joback Method
dvisc	0.0001024	Pa×s	659.60	Joback Method
dvisc	0.0002195	Pa×s	582.25	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=U355896&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