Sebacic acid, isohexyl 3-phenylallyl ester

Inchi: InChI=1S/C25H38O4/c1-22(2)14-12-20-28-24(26)18-10-5-3-4-6-11-19-25(27)29-21-13-1
InchiKey: FYZOFBDADLGRQX-GHRIWEEISA-N
Formula: C25H38O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 402.57

Physical Properties

Property code	Value	Unit	Source
gf	-118.03	kJ/mol	Joback Method
hf	-700.46	kJ/mol	Joback Method
hfus	56.80	kJ/mol	Joback Method
hvap	91.40	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.343		Crippen Method
mcvol	349.930	ml/mol	McGowan Method
pc	1017.48	kPa	Joback Method
rinpol	3071.00		NIST Webbook
rinpol	3071.00		NIST Webbook
tb	954.38	K	Joback Method
tc	1169.02	K	Joback Method
tf	522.17	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.14	J/mol×K	954.38	Joback Method
cpg	1171.13	J/mol×K	990.15	Joback Method
cpg	1186.82	J/mol×K	1025.93	Joback Method
cpg	1201.27	J/mol×K	1061.70	Joback Method
cpg	1214.54	J/mol×K	1097.48	Joback Method
cpg	1226.70	J/mol×K	1133.25	Joback Method
cpg	1237.82	J/mol×K	1169.02	Joback Method
dvisc	0.0004126	Pa×s	522.17	Joback Method

dvisc	0.0001853	Pa×s	594.20	Joback Method
dvisc	0.0000989	Pa×s	666.24	Joback Method
dvisc	0.0000597	Pa×s	738.27	Joback Method
dvisc	0.0000394	Pa×s	810.31	Joback Method
dvisc	0.0000278	Pa×s	882.34	Joback Method
dvisc	0.0000207	Pa×s	954.38	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=U355891&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