Sebacic acid, isohexyl 3-phenylpropyl ester

Inchi: InChI=1S/C25H40O4/c1-22(2)14-12-20-28-24(26)18-10-5-3-4-6-11-19-25(27)29-21-13-1
InchiKey: JPUQHBNBJJJZGU-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)OCCCc1ccccc1
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-198.25	kJ/mol	Joback Method
hf	-817.68	kJ/mol	Joback Method
hfus	56.60	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.263		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	3045.00		NIST Webbook
rinpol	3045.00		NIST Webbook
tb	950.22	K	Joback Method
tc	1163.44	K	Joback Method
tf	527.25	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.25	J/mol×K	950.22	Joback Method
cpg	1199.60	J/mol×K	985.76	Joback Method
cpg	1215.52	J/mol×K	1021.29	Joback Method
cpg	1230.06	J/mol×K	1056.83	Joback Method
cpg	1243.26	J/mol×K	1092.36	Joback Method
cpg	1255.17	J/mol×K	1127.90	Joback Method
cpg	1265.85	J/mol×K	1163.44	Joback Method
dvisc	0.0004436	Pa×s	527.25	Joback Method

dvisc	0.0002040	Pa×s	597.75	Joback Method
dvisc	0.0001106	Pa×s	668.24	Joback Method
dvisc	0.0000673	Pa×s	738.73	Joback Method
dvisc	0.0000447	Pa×s	809.23	Joback Method
dvisc	0.0000317	Pa×s	879.72	Joback Method
dvisc	0.0000237	Pa×s	950.22	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=U354389&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