Sebacic acid, isohexyl 2-phenylphenyl ester

Inchi: InChI=1S/C28H38O4/c1-23(2)15-14-22-31-27(29)20-10-5-3-4-6-11-21-28(30)32-26-19-1
InchiKey: YZWNUXDMZDWYCK-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1-c1ccccc1
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-70.21	kJ/mol	Joback Method
hf	-654.54	kJ/mol	Joback Method
hfus	58.02	kJ/mol	Joback Method
hvap	101.06	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.359		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	3249.00		NIST Webbook
rinpol	3249.00		NIST Webbook
tb	1050.52	K	Joback Method
tc	1286.15	K	Joback Method
tf	600.00	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1260.78	J/mol×K	1050.52	Joback Method
cpg	1275.50	J/mol×K	1089.79	Joback Method
cpg	1288.62	J/mol×K	1129.06	Joback Method
cpg	1300.21	J/mol×K	1168.34	Joback Method
cpg	1310.36	J/mol×K	1207.61	Joback Method
cpg	1319.15	J/mol×K	1246.88	Joback Method
cpg	1326.66	J/mol×K	1286.15	Joback Method
dvisc	0.0002284	Pa×s	600.00	Joback Method

dvisc	0.0001143	Pa×s	675.09	Joback Method
dvisc	0.0000657	Pa×s	750.17	Joback Method
dvisc	0.0000417	Pa×s	825.26	Joback Method
dvisc	0.0000286	Pa×s	900.35	Joback Method
dvisc	0.0000208	Pa×s	975.43	Joback Method
dvisc	0.0000158	Pa×s	1050.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355066&Units=SI
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

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