Sebacic acid, (2-(cyclohexenyl-3)-1-phenyl)ethyl pentyl ester

Inchi: InChI=1S/C29H44O4/c1-2-3-16-23-32-28(30)21-14-6-4-5-7-15-22-29(31)33-27(26-19-12
InchiKey: MQNSQJOOPWIYPI-UHFFFAOYSA-N
Formula: C29H44O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 456.66

Physical Properties

Property code	Value	Unit	Source
gf	-110.16	kJ/mol	Joback Method
hf	-788.14	kJ/mol	Joback Method
hfus	60.01	kJ/mol	Joback Method
hvap	101.07	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.872		Crippen Method
mcvol	395.430	ml/mol	McGowan Method
pc	901.80	kPa	Joback Method
rinpol	3390.00		NIST Webbook
tb	1060.45	K	Joback Method
tc	1298.76	K	Joback Method
tf	580.47	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.78	J/mol×K	1060.45	Joback Method
cpg	1411.02	J/mol×K	1100.17	Joback Method
cpg	1425.41	J/mol×K	1139.89	Joback Method
cpg	1438.03	J/mol×K	1179.60	Joback Method
cpg	1448.98	J/mol×K	1219.32	Joback Method
cpg	1458.35	J/mol×K	1259.04	Joback Method
cpg	1466.23	J/mol×K	1298.76	Joback Method
dvisc	0.0002933	Pa×s	580.47	Joback Method
dvisc	0.0001306	Pa×s	660.47	Joback Method

dvisc	0.0000693	Pa×s	740.46	Joback Method
dvisc	0.0000416	Pa×s	820.46	Joback Method
dvisc	0.0000273	Pa×s	900.46	Joback Method
dvisc	0.0000192	Pa×s	980.45	Joback Method
dvisc	0.0000143	Pa×s	1060.45	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=U354420&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