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

Inchi: InChI=1S/C28H42O4/c1-23(2)22-31-27(29)19-13-5-3-4-6-14-20-28(30)32-26(25-17-11-8

InchiKey: UWCLDSINFMYUNH-UHFFFAOYSA-N

Formula: C28H42O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1

Mol. weight [g/mol]: 442.63

Physical Properties

Property code	Value	Unit	Source
gf	-121.02	kJ/mol	Joback Method
hf	-772.78	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	98.45	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.337		Crippen Method
mcvol	381.340	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	3238.00		NIST Webbook
tb	1037.13	K	Joback Method
tc	1269.86	K	Joback Method
tf	554.20	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.42	J/mol×K	1037.13	Joback Method
cpg	1348.54	J/mol×K	1075.92	Joback Method
cpg	1362.87	J/mol×K	1114.71	Joback Method
cpg	1375.50	J/mol×K	1153.50	Joback Method
cpg	1386.49	J/mol×K	1192.29	Joback Method
cpg	1395.94	J/mol×K	1231.08	Joback Method
cpg	1403.92	J/mol×K	1269.86	Joback Method
dvisc	0.0003761	Pa×s	554.20	Joback Method
dvisc	0.0001569	Pa×s	634.69	Joback Method

dvisc	0.0000797	Pa×s	715.18	Joback Method
dvisc	0.0000464	Pa×s	795.67	Joback Method
dvisc	0.0000299	Pa×s	876.15	Joback Method
dvisc	0.0000207	Pa×s	956.64	Joback Method
dvisc	0.0000152	Pa×s	1037.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354418&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