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

Inchi: InChI=1S/C31H48O4/c1-2-3-4-9-18-25-34-30(32)23-16-7-5-6-8-17-24-31(33)35-29(28-21
InchiKey: MILKMTREHOOLNX-UHFFFAOYSA-N
Formula: C31H48O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]: 484.71

Physical Properties

Property code	Value	Unit	Source
gf	-93.32	kJ/mol	Joback Method
hf	-829.42	kJ/mol	Joback Method
hfus	65.19	kJ/mol	Joback Method
hvap	105.52	kJ/mol	Joback Method
log10ws	-9.59		Crippen Method
logp	8.652		Crippen Method
mcvol	423.610	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3613.00		NIST Webbook
tb	1106.21	K	Joback Method
tc	1359.35	K	Joback Method
tf	603.01	K	Joback Method
vc	1.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.77	J/mol×K	1106.21	Joback Method
cpg	1537.20	J/mol×K	1148.40	Joback Method
cpg	1551.56	J/mol×K	1190.59	Joback Method
cpg	1563.98	J/mol×K	1232.78	Joback Method
cpg	1574.57	J/mol×K	1274.97	Joback Method
cpg	1583.47	J/mol×K	1317.16	Joback Method
cpg	1590.79	J/mol×K	1359.35	Joback Method
dvisc	0.0002226	Pa×s	603.01	Joback Method
dvisc	0.0000977	Pa×s	686.88	Joback Method

dvisc	0.0000513	Pa×s	770.74	Joback Method
dvisc	0.0000306	Pa×s	854.61	Joback Method
dvisc	0.0000200	Pa×s	938.48	Joback Method
dvisc	0.0000140	Pa×s	1022.34	Joback Method
dvisc	0.0000104	Pa×s	1106.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354423&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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