

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

Inchi:	InChI=1S/C30H46O4/c1-2-3-4-17-24-33-29(31)22-15-7-5-6-8-16-23-30(32)34-28(27-20-
InchiKey:	KBCSUJJOXIGHJPX-UHFFFAOYSA-N
Formula:	C30H46O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]:	470.68

Physical Properties

Property code	Value	Unit	Source
gf	-101.74	kJ/mol	Joback Method
hf	-808.78	kJ/mol	Joback Method
hfus	62.60	kJ/mol	Joback Method
hvap	103.30	kJ/mol	Joback Method
log10ws	-9.17		Crippen Method
logp	8.262		Crippen Method
mcvol	409.520	ml/mol	McGowan Method
pc	851.97	kPa	Joback Method
rmpol	3490.00		NIST Webbook
tb	1083.33	K	Joback Method
tc	1328.42	K	Joback Method
tf	591.74	K	Joback Method
vc	1.569	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.66	J/molxK	1083.33	Joback Method
cpg	1473.98	J/molxK	1124.18	Joback Method
cpg	1488.35	J/molxK	1165.03	Joback Method
cpg	1500.87	J/molxK	1205.87	Joback Method
cpg	1511.64	J/molxK	1246.72	Joback Method
cpg	1520.78	J/molxK	1287.57	Joback Method
cpg	1528.39	J/molxK	1328.42	Joback Method
dvisc	0.0002558	Paxs	591.74	Joback Method
dvisc	0.0001131	Paxs	673.67	Joback Method

dvisc	0.0000597	Paxs	755.60	Joback Method
dvisc	0.0000357	Paxs	837.53	Joback Method
dvisc	0.0000234	Paxs	919.47	Joback Method
dvisc	0.0000164	Paxs	1001.40	Joback Method
dvisc	0.0000122	Paxs	1083.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U354422&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

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