Glutaric acid, 1-phenyl-2-(3-cyclohexenyl)ethyl undecyl ester

Inchi: InChI=1S/C30H46O4/c1-2-3-4-5-6-7-8-9-16-24-33-29(31)22-17-23-30(32)34-28(27-20-14
InchiKey: VXHJBXSHPITMHP-UHFFFAOYSA-N
Formula: C30H46O4
SMILES: CCCCCCCCCCCOC(=O)CCCC(=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
rinpol	3478.00		NIST Webbook
tb	1083.33	K	Joback Method
tc	1328.42	K	Joback Method
tf	591.74	K	Joback Method
vc	1.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.66	J/mol×K	1083.33	Joback Method
cpg	1520.78	J/mol×K	1287.57	Joback Method
cpg	1511.64	J/mol×K	1246.72	Joback Method
cpg	1500.87	J/mol×K	1205.87	Joback Method
cpg	1488.35	J/mol×K	1165.03	Joback Method
cpg	1473.98	J/mol×K	1124.18	Joback Method
cpg	1528.39	J/mol×K	1328.42	Joback Method
dvisc	0.0000122	Pa×s	1083.33	Joback Method
dvisc	0.0000164	Pa×s	1001.40	Joback Method

dvisc	0.0000234	Pa×s	919.47	Joback Method
dvisc	0.0000357	Pa×s	837.53	Joback Method
dvisc	0.0000597	Pa×s	755.60	Joback Method
dvisc	0.0001131	Pa×s	673.67	Joback Method
dvisc	0.0002558	Pa×s	591.74	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=U358594&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