

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

Inchi:	InChI=1S/C31H48O4/c1-2-3-4-5-6-7-8-9-10-17-25-34-30(32)23-18-24-31(33)35-29(28-2
InchiKey:	CFXJMBINCWFHSX-UHFFFAOYSA-N
Formula:	C31H48O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=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
mvol	423.610	ml/mol	McGowan Method
pc	806.16	kPa	Joback Method
rinpol	3601.00		NIST Webbook
rinpol	3601.00		NIST Webbook
tb	1106.21	K	Joback Method
tc	1359.35	K	Joback Method
tf	603.01	K	Joback Method
vc	1.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.77	J/molxK	1106.21	Joback Method
cpg	1537.20	J/molxK	1148.40	Joback Method
cpg	1551.56	J/molxK	1190.59	Joback Method
cpg	1563.98	J/molxK	1232.78	Joback Method
cpg	1574.57	J/molxK	1274.97	Joback Method
cpg	1583.47	J/molxK	1317.16	Joback Method
cpg	1590.79	J/molxK	1359.35	Joback Method
dvisc	0.0002226	Paxs	603.01	Joback Method

dvisc	0.0000977	Paxs	686.88	Joback Method
dvisc	0.0000513	Paxs	770.74	Joback Method
dvisc	0.0000306	Paxs	854.61	Joback Method
dvisc	0.0000200	Paxs	938.48	Joback Method
dvisc	0.0000140	Paxs	1022.34	Joback Method
dvisc	0.0000104	Paxs	1106.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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