Glutaric acid, dodec-2-en-1-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C24H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-18-28-23(26)14-13-15-24(27)29-22-17

InchiKey: CLZMXCFZEBRJNG-VAWYXSNFSA-N

Formula: C24H35ClO4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 422.99

Physical Properties

Property code	Value	Unit	Source
gf	-155.20	kJ/mol	Joback Method
hf	-713.22	kJ/mol	Joback Method
hfus	61.15	kJ/mol	Joback Method
hvap	95.27	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.964		Crippen Method
mcvol	348.080	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		NIST Webbook
tb	979.33	K	Joback Method
tc	1199.27	K	Joback Method
tf	580.86	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.75	J/mol×K	979.33	Joback Method
cpg	1181.71	J/mol×K	1162.61	Joback Method
cpg	1171.08	J/mol×K	1125.95	Joback Method
cpg	1159.32	J/mol×K	1089.30	Joback Method
cpg	1146.38	J/mol×K	1052.64	Joback Method
cpg	1132.21	J/mol×K	1015.99	Joback Method
cpg	1191.26	J/mol×K	1199.27	Joback Method
dvisc	0.0000234	Pa×s	979.33	Joback Method

dvisc	0.0000301	Pa×s	912.92	Joback Method
dvisc	0.0000402	Pa×s	846.51	Joback Method
dvisc	0.0000565	Pa×s	780.10	Joback Method
dvisc	0.0000846	Pa×s	713.68	Joback Method
dvisc	0.0001377	Pa×s	647.27	Joback Method
dvisc	0.0002504	Pa×s	580.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392080&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