Glutaric acid, 3,4-dimethylcyclohexyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C25H44O4/c1-4-5-6-7-8-9-10-11-12-13-19-28-24(26)15-14-16-25(27)29-23-18

InchiKey: LBLKYXKNAWCXTQ-OUKQBFOZSA-N

Formula: C25H44O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)OC1CCC(C)C(C)C1

Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-218.97	kJ/mol	Joback Method
hf	-918.07	kJ/mol	Joback Method
hfus	60.26	kJ/mol	Joback Method
hvap	89.33	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.765		Crippen Method
mcvol	362.830	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	938.35	K	Joback Method
tc	1148.99	K	Joback Method
tf	509.65	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.51	J/mol×K	938.35	Joback Method
cpg	1278.17	J/mol×K	973.46	Joback Method
cpg	1296.20	J/mol×K	1008.56	Joback Method
cpg	1312.62	J/mol×K	1043.67	Joback Method
cpg	1327.49	J/mol×K	1078.77	Joback Method
cpg	1340.84	J/mol×K	1113.88	Joback Method
cpg	1352.72	J/mol×K	1148.99	Joback Method
dvisc	0.0005915	Pa×s	509.65	Joback Method

dvisc	0.0002864	Pa×s	581.10	Joback Method
dvisc	0.0001626	Pa×s	652.55	Joback Method
dvisc	0.0001032	Pa×s	724.00	Joback Method
dvisc	0.0000711	Pa×s	795.45	Joback Method
dvisc	0.0000520	Pa×s	866.90	Joback Method
dvisc	0.0000400	Pa×s	938.35	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=U405434&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