Glutaric acid, di(myrtenyl) ester

Inchi: InChI=1S/C25H36O4/c1-24(2)18-10-8-16(20(24)12-18)14-28-22(26)6-5-7-23(27)29-15-1
InchiKey: IPAYWXFLWLCLLO-UHFFFAOYSA-N
Formula: C25H36O4
SMILES: CC1(C)C2CC=C(COC(=O)CCCC(=O)OCC3=CCC4CC3C4(C)C)C1C2
Mol. weight [g/mol]: 400.55

Physical Properties

Property code	Value	Unit	Source
gf	-75.16	kJ/mol	Joback Method
hf	-687.63	kJ/mol	Joback Method
hfus	45.63	kJ/mol	Joback Method
hvap	88.54	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.228		Crippen Method
mcvol	325.950	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	958.90	K	Joback Method
tc	1183.19	K	Joback Method
tf	646.43	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1175.84	J/mol×K	958.90	Joback Method
cpg	1203.18	J/mol×K	996.28	Joback Method
cpg	1231.39	J/mol×K	1033.66	Joback Method
cpg	1260.79	J/mol×K	1071.04	Joback Method
cpg	1291.68	J/mol×K	1108.42	Joback Method
cpg	1324.37	J/mol×K	1145.81	Joback Method
cpg	1359.18	J/mol×K	1183.19	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=U405546&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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