Glutaric acid, myrtenyl dec-2-yl ester

Inchi: InChI=1S/C25H42O4/c1-5-6-7-8-9-10-12-19(2)29-24(27)14-11-13-23(26)28-18-20-15-16
InchiKey: FRCFUZJNIZONDC-UHFFFAOYSA-N
Formula: C25H42O4
SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 406.60

Physical Properties

Property code	Value	Unit	Source
gf	-194.13	kJ/mol	Joback Method
hf	-873.56	kJ/mol	Joback Method
hfus	52.33	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.375		Crippen Method
mcvol	351.970	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	941.00	K	Joback Method
tc	1152.68	K	Joback Method
tf	566.13	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1227.83	J/mol×K	941.00	Joback Method
cpg	1250.56	J/mol×K	976.28	Joback Method
cpg	1272.84	J/mol×K	1011.56	Joback Method
cpg	1294.80	J/mol×K	1046.84	Joback Method
cpg	1316.61	J/mol×K	1082.12	Joback Method
cpg	1338.42	J/mol×K	1117.40	Joback Method
cpg	1360.37	J/mol×K	1152.68	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=U405544&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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