Glutaric acid, myrtenyl hept-2-yl ester

Inchi: InChI=1S/C22H36O4/c1-5-6-7-9-16(2)26-21(24)11-8-10-20(23)25-15-17-12-13-18-14-19
InchiKey: XLHBWRKUCOTMRG-UHFFFAOYSA-N
Formula: C22H36O4
SMILES: CCCCCC(C)OC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-219.39	kJ/mol	Joback Method
hf	-811.64	kJ/mol	Joback Method
hfus	44.56	kJ/mol	Joback Method
hvap	81.98	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.204		Crippen Method
mcvol	309.700	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2411.00		NIST Webbook
rinpol	2411.00		NIST Webbook
tb	872.36	K	Joback Method
tc	1075.99	K	Joback Method
tf	532.32	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.31	J/mol×K	872.36	Joback Method
cpg	1056.78	J/mol×K	906.30	Joback Method
cpg	1076.69	J/mol×K	940.24	Joback Method
cpg	1096.18	J/mol×K	974.17	Joback Method
cpg	1115.37	J/mol×K	1008.11	Joback Method
cpg	1134.39	J/mol×K	1042.05	Joback Method
cpg	1153.37	J/mol×K	1075.99	Joback Method

Sources

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=U405541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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