Glutaric acid, myrtenyl 2-ethylhexyl ester

Inchi: InChI=1S/C23H38O4/c1-5-7-9-17(6-2)15-26-21(24)10-8-11-22(25)27-16-18-12-13-19-14
InchiKey: MUXWMNPKPQQYGZ-UHFFFAOYSA-N
Formula: C23H38O4
SMILES: CCCCC(CC)COC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-210.97	kJ/mol	Joback Method
hf	-832.28	kJ/mol	Joback Method
hfus	47.15	kJ/mol	Joback Method
hvap	84.21	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.452		Crippen Method
mcvol	323.790	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	895.24	K	Joback Method
tc	1100.70	K	Joback Method
tf	543.59	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.25	J/mol×K	895.24	Joback Method
cpg	1120.39	J/mol×K	929.48	Joback Method
cpg	1140.99	J/mol×K	963.73	Joback Method
cpg	1161.21	J/mol×K	997.97	Joback Method
cpg	1181.17	J/mol×K	1032.21	Joback Method
cpg	1201.01	J/mol×K	1066.46	Joback Method
cpg	1220.85	J/mol×K	1100.70	Joback Method

Sources

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=U405542&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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