Glutaric acid, myrtenyl 8-chlorooctyl ester

Inchi: InChI=1S/C23H37ClO4/c1-23(2)19-13-12-18(20(23)16-19)17-28-22(26)11-9-10-21(25)27
InchiKey: APPBDYAQVBBBNQ-UHFFFAOYSA-N
Formula: C23H37ClO4
SMILES: CC1(C)C2CC=C(COC(=O)CCCC(=O)OCCCCCCCCCCl)C1C2
Mol. weight [g/mol]: 412.99

Physical Properties

Property code	Value	Unit	Source
gf	-220.46	kJ/mol	Joback Method
hf	-842.74	kJ/mol	Joback Method
hfus	54.87	kJ/mol	Joback Method
hvap	88.98	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.815		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1072.87	kPa	Joback Method
rinpol	2970.00		NIST Webbook
rinpol	2970.00		NIST Webbook
tb	933.11	K	Joback Method
tc	1144.23	K	Joback Method
tf	588.51	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.71	J/mol×K	933.11	Joback Method
cpg	1151.61	J/mol×K	968.30	Joback Method
cpg	1172.15	J/mol×K	1003.48	Joback Method
cpg	1192.47	J/mol×K	1038.67	Joback Method
cpg	1212.72	J/mol×K	1073.86	Joback Method
cpg	1233.03	J/mol×K	1109.05	Joback Method
cpg	1253.57	J/mol×K	1144.23	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=U405545&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