Glutaric acid, myrtenyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C21H34O4/c1-6-18(14(2)3)25-20(23)9-7-8-19(22)24-13-15-10-11-16-12-17(15
InchiKey: QBQDMMHIMWCVRZ-UHFFFAOYSA-N
Formula: C21H34O4
SMILES: CCC(OC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C)C(C)C
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-230.25	kJ/mol	Joback Method
hf	-796.28	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	79.37	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.670		Crippen Method
mcvol	295.610	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	849.04	K	Joback Method
tc	1053.41	K	Joback Method
tf	506.05	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.78	J/mol×K	849.04	Joback Method
cpg	994.81	J/mol×K	883.10	Joback Method
cpg	1014.24	J/mol×K	917.16	Joback Method
cpg	1033.19	J/mol×K	951.23	Joback Method
cpg	1051.80	J/mol×K	985.29	Joback Method
cpg	1070.18	J/mol×K	1019.35	Joback Method
cpg	1088.46	J/mol×K	1053.41	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=U405539&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