Glutaric acid, myrtenyl cyclohexylmethyl ester

Inchi: InChI=1S/C22H34O4/c1-22(2)18-12-11-17(19(22)13-18)15-26-21(24)10-6-9-20(23)25-14
InchiKey: SRNKJFHDUOJIHW-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CC1(C)C2CC=C(COC(=O)CCCC(=O)OCC3CCCCC3)C1C2
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-192.50	kJ/mol	Joback Method
hf	-752.04	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.816		Crippen Method
mcvol	298.840	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	892.35	K	Joback Method
tc	1111.08	K	Joback Method
tf	554.70	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.40	J/mol×K	892.35	Joback Method
cpg	1054.98	J/mol×K	928.80	Joback Method
cpg	1075.89	J/mol×K	965.26	Joback Method
cpg	1096.29	J/mol×K	1001.71	Joback Method
cpg	1116.34	J/mol×K	1038.17	Joback Method
cpg	1136.20	J/mol×K	1074.62	Joback Method
cpg	1156.03	J/mol×K	1111.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405543&Units=SI
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

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