Succinic acid, cyclohexylmethyl neryl ester

Inchi: InChI=1S/C21H34O4/c1-17(2)8-7-9-18(3)14-15-24-20(22)12-13-21(23)25-16-19-10-5-4-6
InchiKey: PDGQJGJZIAJVRG-JXAWBTAJSA-N
Formula: C21H34O4
SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OCC1CCCCC1
Mol. weight [g/mol]: 350.49

Physical Properties

Property code	Value	Unit	Source
gf	-174.11	kJ/mol	Joback Method
hf	-697.19	kJ/mol	Joback Method
hfus	45.34	kJ/mol	Joback Method
hvap	81.16	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.126		Crippen Method
mcvol	302.170	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	860.09	K	Joback Method
tc	1067.62	K	Joback Method
tf	440.05	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.18	J/mol×K	860.09	Joback Method
cpg	992.59	J/mol×K	894.68	Joback Method
cpg	1009.75	J/mol×K	929.27	Joback Method
cpg	1025.70	J/mol×K	963.86	Joback Method
cpg	1040.51	J/mol×K	998.44	Joback Method
cpg	1054.22	J/mol×K	1033.03	Joback Method
cpg	1066.90	J/mol×K	1067.62	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=U391242&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