Succinic acid, hept-2-yl neryl ester

Inchi: InChI=1S/C21H36O4/c1-6-7-8-12-19(5)25-21(23)14-13-20(22)24-16-15-18(4)11-9-10-17
InchiKey: UGZADRPOGUMZED-SDXDJHTJSA-N
Formula: C21H36O4
SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 352.51

Physical Properties

Property code	Value	Unit	Source
gf	-201.00	kJ/mol	Joback Method
hf	-756.79	kJ/mol	Joback Method
hfus	49.98	kJ/mol	Joback Method
hvap	80.34	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.514		Crippen Method
mcvol	313.030	ml/mol	McGowan Method
pc	1096.44	kPa	Joback Method
rinpol	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	840.10	K	Joback Method
tc	1034.15	K	Joback Method
tf	417.67	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.21	J/mol×K	840.10	Joback Method
cpg	996.00	J/mol×K	872.44	Joback Method
cpg	1012.76	J/mol×K	904.78	Joback Method
cpg	1028.55	J/mol×K	937.13	Joback Method
cpg	1043.41	J/mol×K	969.47	Joback Method
cpg	1057.37	J/mol×K	1001.81	Joback Method
cpg	1070.48	J/mol×K	1034.15	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=U391239&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