Succinic acid, 3-methylbut-2-en-1-yl neryl ester

Inchi: InChI=1S/C19H30O4/c1-15(2)7-6-8-17(5)12-14-23-19(21)10-9-18(20)22-13-11-16(3)4/h7

InchiKey: FBCUFTYQYAQVRQ-ATVHPVEESA-N

Formula: C19H30O4

SMILES: CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-143.73	kJ/mol	Joback Method
hf	-602.80	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	76.31	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.512		Crippen Method
mcvol	280.550	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	798.82	K	Joback Method
tc	994.13	K	Joback Method
tf	391.09	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.72	J/mol×K	798.82	Joback Method
cpg	849.32	J/mol×K	831.37	Joback Method
cpg	865.02	J/mol×K	863.92	Joback Method
cpg	879.87	J/mol×K	896.48	Joback Method
cpg	893.93	J/mol×K	929.03	Joback Method
cpg	907.23	J/mol×K	961.58	Joback Method
cpg	919.84	J/mol×K	994.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391237&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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