Succinic acid, di(neryl) ester

Inchi: InChI=1S/C24H38O4/c1-19(2)9-7-11-21(5)15-17-27-23(25)13-14-24(26)28-18-16-22(6)12-10-8-20(3)4/h9-10,15-16H,7-8,11-14,17-18H2,1-6H3/b21-15+,22-16+

InchiKey: WCOGJMOUNVGCLA-BMJUYKDLSA-N

Formula: C24H38O4

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

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-29.96	kJ/mol	Joback Method
hf	-598.57	kJ/mol	Joback Method
hfus	59.06	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.238		Crippen Method
mcvol	346.700	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	2675.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tb	917.26	K	Joback Method
tc	1125.05	K	Joback Method
tf	428.40	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.09	J/mol×K	917.26	Joback Method
cpg	1125.32	J/mol×K	951.89	Joback Method
cpg	1142.63	J/mol×K	986.52	Joback Method
cpg	1159.10	J/mol×K	1021.15	Joback Method
cpg	1174.82	J/mol×K	1055.78	Joback Method
cpg	1189.87	J/mol×K	1090.42	Joback Method
cpg	1204.33	J/mol×K	1125.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391244&Units=SI

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