

Succinic acid, dec-2-yl neryl ester

Inchi:

lnchl=1S/C24H42O4/c1-6-7-8-9-10-11-15-22(5)28-24(26)17-16-23(25)27-19-18-21(4)14

InchiKey:

BYZDCZADYGLTRK-UZYVYHOESA-N

Formula:

C24H42O4

SMILES:

CCCCCCCCC(C)OC(=O)CCC(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]:

394.59

Physical Properties

Property code	Value	Unit	Source
gf	-175.74	kJ/mol	Joback Method
hf	-818.71	kJ/mol	Joback Method
hfus	57.75	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.685		Crippen Method
mcvol	355.300	ml/mol	McGowan Method
pc	913.84	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	908.74	K	Joback Method
tc	1112.69	K	Joback Method
tf	451.48	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.03	J/mol×K	908.74	Joback Method
cpg	1182.01	J/mol×K	942.73	Joback Method
cpg	1199.83	J/mol×K	976.72	Joback Method
cpg	1216.53	J/mol×K	1010.71	Joback Method
cpg	1232.18	J/mol×K	1044.71	Joback Method
cpg	1246.83	J/mol×K	1078.70	Joback Method
cpg	1260.55	J/mol×K	1112.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391243&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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