

Sclareolide

Other names:	Naphtho[2,1-b]furan-2(1H)-one, decahydro-3a,6,6,9a-tetramethyl-, [3aR-(3a«alpha»,5a«beta»,9a«alpha»,9b«beta»)]-Naphtho[2,1-b]furan-2(1H)-one, 3a,4,5,5a«alpha»,6,7,8,9,9a,9b«alpha»-decahydro-3a«beta»,6,6,9a«beta»-tetramethyl-(+)-Norambreinolide Decahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan-2(1H)-one Norambreinolid Norambreinolide Naphtho[2,1-b]furan-2(1H)-one, decahydro-3a,6,6,9a-tetramethyl-, (3aR,5aS,9aS,9bR)-(+)-Sclareolide [3aR-(3a«alpha»,5a«beta»,9a«alpha»,9b«beta»)]decahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan-2(1H)-one
Inchi:	InChI=1S/C16H26O2/c1-14(2)7-5-8-15(3)11(14)6-9-16(4)12(15)10-13(17)18-16/h11-12H
InchiKey:	IMKJGXCIJJXALX-UHFFFAOYSA-N
Formula:	C16H26O2
SMILES:	CC1(C)CCCC2(C)C1CCC1(C)OC(=O)CC12
Mol. weight [g/mol]:	250.38
CAS:	564-20-5

Physical Properties

Property code	Value	Unit	Source
gf	-22.91	kJ/mol	Joback Method
hf	-444.47	kJ/mol	Joback Method
hfus	13.94	kJ/mol	Joback Method
hvap	56.32	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.935		Crippen Method
mcvol	211.160	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2089.00		NIST Webbook
tb	688.93	K	Joback Method
tc	940.93	K	Joback Method
tf	467.83	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.19	J/mol×K	688.93	Joback Method
cpg	682.03	J/mol×K	730.93	Joback Method
cpg	706.17	J/mol×K	772.93	Joback Method
cpg	730.10	J/mol×K	814.93	Joback Method
cpg	754.28	J/mol×K	856.93	Joback Method
cpg	779.20	J/mol×K	898.93	Joback Method
cpg	805.34	J/mol×K	940.93	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=C564205&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
mccvol:	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

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