Lapachol

Other names:	1,4-Naphthalenedione, 2-hydroxy-3-(3-methyl-2-butenyl)-
	1,4-Naphthoquinone, 2-hydroxy-3-(3-methyl-2-butenyl)-
	Bethabarra Wood
	C.I. Natural Yellow 16
	C.I. 75490
	Greenhartin
	Ipe-Tobacco Wood
	Lapachol Wood
	NSC 11905
	Surinam Greenheart Wood
	Taigu Wood
	Taiguic acid
	Tecomin
	2-Hydroxy-3-(3-methyl-2-butenyl)-1,4-naphthoquinone
	Greenharten
	2-Hydroxy-3-(3-methyl-2-butenyl)-1,4-naphthalenedione
	Lapachic acid
	Zlut prirodni 16
	NSC 629756
	2-hydroxy-3-(3-methylbut-2-enyl)-1,4-naphthoquinone
Inchi:	InChI=1S/C15H14O3/c1-9(2)7-8-12-13(16)10-5-3-4-6-11(10)14(17)15(12)18/h3-7,18H,8H
InchiKey:	CIEYTVIYYGTCCI-UHFFFAOYSA-N
Formula:	C15H14O3
SMILES:	CC(C)=CCC1=C(O)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	242.27
CAS:	84-79-7

Physical Properties

Property code	Value	Unit	Source
gf	-65.07	kJ/mol	Joback Method
hf	-326.25	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.234		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method

tb	830.92	K	Joback Method
tc	1064.27	K	Joback Method
tf	520.43	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.11	J/mol×K	830.92	Joback Method
cpg	560.58	J/mol×K	869.81	Joback Method
cpg	572.05	J/mol×K	908.70	Joback Method
cpg	582.55	J/mol×K	947.59	Joback Method
cpg	592.09	J/mol×K	986.48	Joback Method
cpg	600.69	J/mol×K	1025.38	Joback Method
cpg	608.36	J/mol×K	1064.27	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84797&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

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

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume