Thymoquinone

Other names:	2,5-Cyclohexadiene-1,4-dione, 2-methyl-5-(1-methylethyl)- 2,5-Cyclohexadiene-1,4-dione, 5-isopropyl-2-methyl- 2-Isopropyl-5-methyl-p-benzoquinone 2-Methyl-5-(1-methylethyl)-2,5-cyclohexadiene-1,4-dione 2-Methyl-5-isopropyl-1,4-benzoquinone 2-Methyl-5-isopropyl-p-benzoquinone 2-isopropyl-5-methyl-1,4-benzoquinone 2-isopropyl-5-methylbenzoquinone 2-isopropyl-5-methylcyclohexa-2,5-diene-1,4-dione 5-Isopropyl-2-methyl-1,4-benzoquinone 5-Isopropyl-2-methyl-p-benzoquinone NSC 2228 Thymoquinon p-Cymene-2,5-dione p-Mentha-3,6-diene-2,5-dione thymolquinone
Inchi:	InChI=1S/C10H12O2/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4-6H,1-3H3
InchiKey:	KEQHJBNSCLWCAE-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC1=CC(=O)C(C(C)C)=CC1=O
Mol. weight [g/mol]:	164.20
CAS:	490-91-5

Physical Properties

Property code	Value	Unit	Source
chs	-5319.10	kJ/mol	NIST Webbook
ea	1.76 ± 0.06	eV	NIST Webbook
gf	-141.48	kJ/mol	Joback Method
hf	-363.13	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.667		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1246.00		NIST Webbook

rinpol	1252.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1248.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1249.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1253.00		NIST Webbook
tb	505.20	K	NIST Webbook
tc	835.62	K	Joback Method
tf	316.70	K	Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds
tf	316.70	K	Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid

vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.48	J/mol×K	795.67	Joback Method
cpg	329.59	J/mol×K	595.90	Joback Method
cpg	345.03	J/mol×K	635.85	Joback Method
cpg	359.68	J/mol×K	675.81	Joback Method
cpg	373.51	J/mol×K	715.76	Joback Method
cpg	386.45	J/mol×K	755.71	Joback Method
cpg	409.53	J/mol×K	835.62	Joback Method
hfust	18.16	kJ/mol	323.20	NIST Webbook

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=C490915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility studies on the system of trihexyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]amide) ionic liquid and pharmaceutical and bioactive compounds in supercritical carbon dioxide: Experimental measurements and predictive modeling with the GC-EoS:	https://www.doi.org/10.1016/j.fluid.2014.10.033
Solubilities of pharmaceutical and bioactive compounds in trihexyl(tetradecyl)phosphonium chloride ionic liquid:	https://www.doi.org/10.1016/j.fluid.2015.03.053
Solubility of three natural coumarin derivatives: Prenylated coumarins with insecticidal activity in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2019.04.011

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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

Latest version available from:
https://www.chemeo.com/cid/85-850-4/Thymoquinone.pdf
Generated by Cheméo on 2025-12-05 15:01:35.495133406 +0000 UTC m=+4695093.025174060.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.