Menadione

Other names:

1,4-Naphthalenedione, 2-methyl-
1,4-Naphthoquinone, 2-methyl-
2-Methyl-1,4-Naphthalenedione
2-Methyl-1,4-naftochinon
2-Methyl-1,4-naphthalendione
2-Methyl-1,4-naphthochinon
2-Methyl-1,4-naphthoquinone
2-Methylnaphthoquinone
3-Methyl-1,4-naphthoquinone
Aquakay
Aquinone
Hemodal
Juva-K
K-Thrombyl
K-Vitan
Kaergona
Kanone
Kappaxan
Kappaxin
Karcon
Kareon
Kativ-G
Kayklot
Kaykot
Kaynone
Kayquinone
Kipca
Kipca-Oil Soluble
Klottone
Koaxin
Kolklot
MNQ
Menadion
Menaphthene
Menaphthon
Menaphthone
Menaphtone
Menaquinone
Menaquinone O
Mitenon

Mitenone
NSC 4170
Panosine
Prokayvit
Synkay
Thyloquinone
USAF EK-5185
Vitamin K0
Vitamin K2(0)
Vitamin K3

Inchi: InChI=1S/C11H8O2/c1-7-6-10(12)8-4-2-3-5-9(8)11(7)13/h2-6H,1H3
InchiKey: MJVAVZPDRWSRRC-UHFFFAOYSA-N
Formula: C11H8O2
SMILES: CC1=CC(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 172.18
CAS: 58-27-5

Physical Properties

Property code	Value	Unit	Source
chs	-5238.00 ± 4.00	kJ/mol	NIST Webbook
ea	1.76 ± 0.06	eV	NIST Webbook
ea	1.75 ± 0.05	eV	NIST Webbook
gf	-23.97	kJ/mol	Joback Method
hf	-187.42	kJ/mol	Joback Method
hfus	12.71	kJ/mol	Joback Method
hvap	52.86	kJ/mol	Joback Method
ie	9.46	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.51	eV	NIST Webbook
log10ws	-3.03		Aqueous Solubility Prediction Method
log10ws	-3.03		Estimated Solubility Method
logp	2.012		Crippen Method
mcvol	130.070	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	259.23		NIST Webbook
rinpol	259.23		NIST Webbook
tb	638.20	K	Joback Method
tc	899.61	K	Joback Method

tf	380.15	K	Measurement and correlation of ternary solid-liquid equilibrium of 2-methyl-1,4-naphthoquinone + phthalic anhydride + acetone system
tf	377.40	K	Aqueous Solubility Prediction Method
tf	376.00 ± 1.00	K	NIST Webbook
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.48	J/mol×K	638.20	Joback Method
cpg	331.61	J/mol×K	681.77	Joback Method
cpg	344.75	J/mol×K	725.34	Joback Method
cpg	356.89	J/mol×K	768.90	Joback Method
cpg	368.02	J/mol×K	812.47	Joback Method
cpg	378.13	J/mol×K	856.04	Joback Method
cpg	387.19	J/mol×K	899.61	Joback Method

Sources

Measurement and correlation of ternary solid-liquid equilibrium of 2-methyl-1,4-naphthoquinone + phthalic anhydride + acetone system:	https://www.doi.org/10.1016/j.fluid.2015.09.019
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solid-Liquid Equilibrium and Phase Diagram for Ternary 2-Methyl-1,4-naphthoquinone + Phthalic Anhydride + 1,4-Dioxane System:	https://www.doi.org/10.1021/acs.jced.7b00609
Solubility of menadione and dichlone in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2016.04.001
Solubilities of 2-Methyl-1,4-naphthoquinone in Water + (Methanol, Ethanol, 1-Propanol, 2-Propanol, 2-Propanone, and 1,4-Dioxane) and Solubilities and Thermodynamic Properties of Vitamin K3 in Benzene, Toluene, Ethylbenzene, o-Xylene, m-Xylene, and p-Xylene from (303.15 to 333.15) K:	https://www.doi.org/10.1021/je7002989
Solubilities of Vitamin K3 in Benzene, Toluene, Ethylbenzene, o-Xylene, m-Xylene, and p-Xylene from (303.15 to 333.15) K:	https://www.doi.org/10.1021/je7003885
Densities and Viscosities of Binary Mixtures of Vitamin K3 with Benzene, Toluene, Methylbenzene, o-Xylene, m-Xylene, and p-Xylene from (303.15 to 333.15) K:	https://www.doi.org/10.1021/je7006549
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58275&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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