1,4-Naphthalenedione, 2-hydroxy-

Other names:	Henna
	1,4-Naphthoquinone, 2-hydroxy-
	C.I. Natural Orange 6
	C.I. 75480
	Flower of Paradise
	Hana
	Lawson
	Lawsone
	Mehendi
	Mendi
	2-Hydroxy-1,4-naphthoquinone
	2-Hydroxynaphthoquinone
	2-Hydroxy-1,4-naphthalenedione
	NSC 27285
	NSC 8625
	2-Hydroxynaphthalene-1,4-dione
Inchi:	InChI=1S/C10H6O3/c11-8-5-9(12)10(13)7-4-2-1-3-6(7)8/h1-5,12H
InchiKey:	CSFWPUWCSPOLJW-UHFFFAOYSA-N
Formula:	C10H6O3
SMILES:	O=C1C=C(O)C(=O)c2ccccc21
Mol. weight [g/mol]:	174.15
CAS:	83-72-7

Physical Properties

Property code	Value	Unit	Source
gf	-169.21	kJ/mol	Joback Method
hf	-319.01	kJ/mol	Joback Method
hfus	14.21	kJ/mol	Joback Method
hvap	67.31	kJ/mol	Joback Method
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	1.508		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
pc	4498.26	kPa	Joback Method
rinpol	1640.00		NIST Webbook

tb	707.50	K	Joback Method
tc	949.48	K	Joback Method
tf	470.60	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.79	J/mol×K	707.50	Joback Method
cpg	324.26	J/mol×K	747.83	Joback Method
cpg	333.93	J/mol×K	788.16	Joback Method
cpg	342.79	J/mol×K	828.49	Joback Method
cpg	350.82	J/mol×K	868.82	Joback Method
cpg	358.02	J/mol×K	909.15	Joback Method
cpg	364.38	J/mol×K	949.48	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=C83727&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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
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