1,4-Naphthalenedione, 2-methoxy-

Other names: 1,4-Naphthoquinone, 2-methoxy-
2-Methoxy-p-naphthoquinone
2-Methoxy-1,4-naphthoquinone
2-Methoxynaphthoquinone
Inchi: InChI=1S/C11H8O3/c1-14-10-6-9(12)7-4-2-3-5-8(7)11(10)13/h2-6H,1H3
InchiKey: OBGBGHKYJAOXRR-UHFFFAOYSA-N
Formula: C11H8O3
SMILES: COC1=CC(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 188.18
CAS: 2348-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-128.97	kJ/mol	Joback Method
hf	-319.64	kJ/mol	Joback Method
hfus	13.90	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	1.596		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	660.62	K	Joback Method
tc	917.34	K	Joback Method
tf	443.28	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.27	J/mol×K	660.62	Joback Method
cpg	355.15	J/mol×K	703.41	Joback Method
cpg	368.07	J/mol×K	746.19	Joback Method

cpg	379.97	J/mol×K	788.98	Joback Method
cpg	390.82	J/mol×K	831.77	Joback Method
cpg	400.58	J/mol×K	874.55	Joback Method
cpg	409.21	J/mol×K	917.34	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=C2348825&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume