2,6-DIMETHYL-P-BENZOQUINONE

Other names:	p-Benzoquinone, 2,6-dimethyl- m-Xyloquinone 2,6-Dimethyl-p-benzoquinone 2,6-Dimethyl-1,4-benzoquinone 2,6-Dimethyl-1,4-quinone 2,6-Dimethylbenzoquinone 2,6-Dimethylquinone 2,6-Xyloquinone 2,6-Dimethylbenzo-1,4-quinone 2,6-Dimethyl-2,5-cyclohexadien-1,4-dione 3,5-Dimethylbenzoquinone NSC 17549 2,6-Dimethyl-2,5-cycloxehadien-1,4-dione
Inchi:	InChI=1S/C8H8O2/c1-5-3-7(9)4-6(2)8(5)10/h3-4H,1-2H3
InchiKey:	SENUUPBBLQWHMF-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC1=CC(=O)C=C(C)C1=O
Mol. weight [g/mol]:	136.15

Physical Properties

Property code	Value	Unit	Source
ea	1.76 ± 0.05	eV	NIST Webbook
ea	1.76 ± 0.06	eV	NIST Webbook
hfus	7.93	kJ/mol	Joback Method
ie	9.63	eV	Cheméo Relay (1.0)
log10ws	-1.10		Cheméo Relay (1.0)
logp	1.031		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
rinpol	1113.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1703.00		NIST Webbook

ripol	1686.00		NIST Webbook
ripol	1681.00		NIST Webbook
tf	362.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.88	J/mol×K	550.58	Joback Method
cpg	249.76	J/mol×K	591.32	Joback Method
cpg	262.12	J/mol×K	632.05	Joback Method
cpg	273.89	J/mol×K	672.79	Joback Method
cpg	285.02	J/mol×K	713.53	Joback Method
cpg	295.44	J/mol×K	754.27	Joback Method
cpg	305.11	J/mol×K	795.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C527617&Units=SI
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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

ripol: Polar retention indices

tf: Normal melting (fusion) point