

2,5-Cyclohexadiene-1,4-dione, 2,3-dimethyl-

Other names:	p-Benzoquinone, 2,3-dimethyl- o-Xyloquinone 2,3-Dimethyl-p-benzoquinone 2,3-Dimethyl-p-quinone 2,3-Dimethyl-1,4-benzoquinone 2,3-Dimethylbenzoquinone 2,3-Dimethylquinone 2,3-Dimethylbenzo-1,4-quinone 2,3-Dimethyl-2,5-cyclohexadiene-1,4-dione NSC 402192
Inchi:	InChI=1S/C8H8O2/c1-5-6(2)8(10)4-3-7(5)9/h3-4H,1-2H3
InchiKey:	AIACLXROWHONEE-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC1=C(C)C(=O)C=CC1=O
Mol. weight [g/mol]:	136.15
CAS:	526-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-155.88	kJ/mol	Joback Method
hf	-316.57	kJ/mol	Joback Method
hfus	7.93	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.031		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	1182.00		NIST Webbook
tb	550.58	K	Joback Method
tc	795.00	K	Joback Method
tf	354.54	K	Joback Method
vc	0.404	m3/kmol	Joback Method

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=C526863&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	http://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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

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