p-Benzoquinone, 1-methoxy-5-hydroxymethyl

Inchi: InChI=1S/C8H8O4/c1-12-8-3-6(10)5(4-9)2-7(8)11/h2-3,9H,4H2,1H3
InchiKey: KTTQYVYUXZOVEN-UHFFFAOYSA-N
Formula: C8H8O4
SMILES: COC1=CC(=O)C(CO)=CC1=O
Mol. weight [g/mol]: 168.15

Physical Properties

Property code	Value	Unit	Source
gf	-397.70	kJ/mol	Joback Method
hf	-601.02	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	63.63	kJ/mol	Joback Method
log10ws	-0.18		Crippen Method
logp	-0.413		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
rinpol	1540.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1573.00		NIST Webbook
tb	665.18	K	Joback Method
tc	885.89	K	Joback Method
tf	437.59	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.51	J/mol×K	665.18	Joback Method
cpg	316.36	J/mol×K	701.97	Joback Method
cpg	326.61	J/mol×K	738.75	Joback Method
cpg	336.20	J/mol×K	775.54	Joback Method
cpg	345.09	J/mol×K	812.32	Joback Method
cpg	353.20	J/mol×K	849.11	Joback Method

cpg	360.49	J/mol×K	885.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R119685&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://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