p-Benzoquinone, methoxy

Inchi: InChI=1S/C7H6O3/c1-10-7-4-5(8)2-3-6(7)9/h2-4H,1H3
InchiKey: ZJKWJHONFFKJHG-UHFFFAOYSA-N
Formula: C7H6O3
SMILES: COC1=CC(=O)C=CC1=O
Mol. weight [g/mol]: 138.12
CAS: 2880-58-2

Physical Properties

Property code	Value	Unit	Source
gf	-259.67	kJ/mol	Joback Method
hf	-416.68	kJ/mol	Joback Method
hfus	6.91	kJ/mol	Joback Method
hvap	44.06	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.225		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1240.00		NIST Webbook
tb	545.14	K	Joback Method
tc	789.90	K	Joback Method
tf	352.98	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.88	J/mol×K	545.14	Joback Method
cpg	227.72	J/mol×K	585.93	Joback Method
cpg	239.12	J/mol×K	626.73	Joback Method
cpg	250.01	J/mol×K	667.52	Joback Method

cpg	260.31	J/mol×K	708.31	Joback Method
cpg	269.95	J/mol×K	749.10	Joback Method
cpg	278.84	J/mol×K	789.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2880582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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