4-methyl-1,2-benzoquinone

Inchi: InChI=1S/C7H6O2/c1-5-2-3-6(8)7(9)4-5/h2-4H,1H3
InchiKey: GYEMOVUSSDZYLQ-UHFFFAOYSA-N
Formula: C7H6O2
SMILES: CC1=CC(=O)C(=O)C=C1
Mol. weight [g/mol]: 122.12
CAS: 4847-64-7

Physical Properties

Property code	Value	Unit	Source
gf	-154.67	kJ/mol	Joback Method
hf	-284.46	kJ/mol	Joback Method
hfus	5.73	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.641		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
ripol	1842.00		NIST Webbook
ripol	1842.00		NIST Webbook
tb	522.72	K	Joback Method
tc	771.09	K	Joback Method
tf	330.75	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.24	J/mol×K	522.72	Joback Method
cpg	206.10	J/mol×K	564.11	Joback Method
cpg	217.49	J/mol×K	605.51	Joback Method
cpg	228.34	J/mol×K	646.90	Joback Method
cpg	238.62	J/mol×K	688.30	Joback Method
cpg	248.26	J/mol×K	729.69	Joback Method
cpg	257.20	J/mol×K	771.09	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=C4847647&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume