2,6-Dimethyl-3-methoxymethyl-p-benzoquinone

Other names: 2,6-Dimethyl-3-(methoxymethyl)-benzoquinone
Inchi: InChI=1S/C10H12O3/c1-6-4-9(11)8(5-13-3)7(2)10(6)12/h4H,5H2,1-3H3
InchiKey: REYIEWLSGQOMMT-UHFFFAOYSA-N
Formula: C10H12O3
SMILES: COCC1=C(C)C(=O)C(C)=CC1=O
Mol. weight [g/mol]: 180.20

Physical Properties

Property code	Value	Unit	Source
gf	-253.67	kJ/mol	Joback Method
hf	-501.54	kJ/mol	Joback Method
hfus	13.90	kJ/mol	Joback Method
hvap	52.07	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.047		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1516.00		NIST Webbook
tb	623.74	K	Joback Method
tc	855.80	K	Joback Method
tf	411.83	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.99	J/mol×K	623.74	Joback Method
cpg	367.66	J/mol×K	662.42	Joback Method
cpg	381.64	J/mol×K	701.09	Joback Method
cpg	394.86	J/mol×K	739.77	Joback Method
cpg	407.25	J/mol×K	778.45	Joback Method
cpg	418.74	J/mol×K	817.13	Joback Method
cpg	429.25	J/mol×K	855.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R274178&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