

Thymohydroquinone

Inchi:	InChI=1S/C10H14O2/c1-6(2)8-5-9(11)7(3)4-10(8)12/h4-6,11-12H,1-3H3
InchiKey:	OQIOHYHRGZNZCW-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	Cc1cc(O)c(C(C)C)cc1O
Mol. weight [g/mol]:	166.22
CAS:	2217-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-175.58	kJ/mol	Joback Method
hf	-384.57	kJ/mol	Joback Method
hfus	23.35	kJ/mol	Joback Method
hvap	66.43	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.530		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1554.70		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1552.00		NIST Webbook
ripol	2178.00		NIST Webbook
ripol	2176.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2178.00		NIST Webbook
tb	620.66	K	Joback Method
tc	855.51	K	Joback Method
tf	449.84	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.48	J/mol×K	620.66	Joback Method
cpg	414.52	J/mol×K	816.37	Joback Method
cpg	404.76	J/mol×K	777.23	Joback Method
cpg	394.62	J/mol×K	738.09	Joback Method
cpg	383.95	J/mol×K	698.94	Joback Method
cpg	372.61	J/mol×K	659.80	Joback Method
cpg	424.02	J/mol×K	855.51	Joback Method
dvisc	0.0000046	Pa×s	620.66	Joback Method
dvisc	0.0000074	Pa×s	592.19	Joback Method
dvisc	0.0000127	Pa×s	563.72	Joback Method
dvisc	0.0000231	Pa×s	535.25	Joback Method
dvisc	0.0000447	Pa×s	506.78	Joback Method
dvisc	0.0000936	Pa×s	478.31	Joback Method
dvisc	0.0002154	Pa×s	449.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2217609&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
dvisc:	Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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