

2,3,4,6-TETRAMETHYLPHENOL

Inchi:	InChI=1S/C10H14O/c1-6-5-7(2)10(11)9(4)8(6)3/h5,11H,1-4H3
InchiKey:	WEJVFHVGNQBRGH-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	Cc1cc(C)c(O)c(C)c1C
Mol. weight [g/mol]:	150.22
CAS:	3238-38-8

Physical Properties

Property code	Value	Unit	Source
af	0.5459		Cheméo Relay (1.0)
gf	-37.78	kJ/mol	Joback Method
hf	-203.97	kJ/mol	Cheméo Relay (1.0)
hfus	20.31	kJ/mol	Joback Method
hvap	78.26	kJ/mol	Cheméo Relay (1.0)
ie	7.72	eV	Cheméo Relay (1.0)
log10ws	-2.29		Cheméo Relay (1.0)
logp	2.626		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	523.15 ± 4.00	K	NIST Webbook
tb	523.15 ± 4.00	K	NIST Webbook
tc	746.65	K	Cheméo Relay (1.0)
tf	353.15 ± 2.00	K	NIST Webbook
vc	0.479	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.51	J/mol×K	550.44	Joback Method
cpg	323.33	J/mol×K	587.39	Joback Method
cpg	335.42	J/mol×K	624.34	Joback Method
cpg	346.83	J/mol×K	661.30	Joback Method
cpg	357.63	J/mol×K	698.25	Joback Method
cpg	367.86	J/mol×K	735.20	Joback Method

cpg	377.60	J/mol×K	772.15	Joback Method
dvisc	0.0010235	Pa×s	378.16	Joback Method
dvisc	0.0005185	Pa×s	406.87	Joback Method
dvisc	0.0002873	Pa×s	435.59	Joback Method
dvisc	0.0001712	Pa×s	464.30	Joback Method
dvisc	0.0001084	Pa×s	493.01	Joback Method
dvisc	0.0000722	Pa×s	521.73	Joback Method
dvisc	0.0000501	Pa×s	550.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54577e+01
Coeff. B	-4.73206e+03
Coeff. C	-8.65860e+01
Temperature range (K), min.	398.52
Temperature range (K), max.	552.97

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3238388&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/76-030-4/2-3-4-6-TETRAMETHYLPHENOL.pdf>

Generated by Cheméo on 2026-07-21 17:50:08.610937755 +0000 UTC m=+167304.452823136.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.