Phenol, 2,3,4-trimethyl-

Other names: 2,3,4-trimethylphenol
Inchi: InChI=1S/C9H12O/c1-6-4-5-9(10)8(3)7(6)2/h4-5,10H,1-3H3
InchiKey: XRUGBBIQLIVCSI-UHFFFAOYSA-N
Formula: C9H12O
SMILES: Cc1ccc(O)c(C)c1C
Mol. weight [g/mol]: 136.19
CAS: 526-85-2

Physical Properties

Property code	Value	Unit	Source
gf	-36.57	kJ/mol	Joback Method
hf	-192.81	kJ/mol	Joback Method
hfus	18.11	kJ/mol	Joback Method
hvap	52.24	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.317		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	509.00 ± 3.00	K	NIST Webbook
tb	510.00 ± 3.00	K	NIST Webbook
tb	509.00 ± 3.00	K	NIST Webbook
tc	747.15	K	Joback Method
tf	354.20 ± 3.00	K	NIST Webbook
tf	354.00 ± 3.00	K	NIST Webbook
tf	354.00 ± 2.00	K	NIST Webbook
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.77	J/mol×K	522.58	Joback Method
cpg	320.54	J/mol×K	709.72	Joback Method
cpg	311.07	J/mol×K	672.29	Joback Method
cpg	301.03	J/mol×K	634.86	Joback Method

cpg	290.34	J/mol×K	597.44	Joback Method
cpg	278.94	J/mol×K	560.01	Joback Method
cpg	329.50	J/mol×K	747.15	Joback Method
dvisc	0.0000662	Pa×s	522.58	Joback Method
dvisc	0.0000978	Pa×s	494.54	Joback Method
dvisc	0.0001515	Pa×s	466.51	Joback Method
dvisc	0.0002482	Pa×s	438.47	Joback Method
dvisc	0.0004351	Pa×s	410.44	Joback Method
dvisc	0.0008278	Pa×s	382.40	Joback Method
dvisc	0.0017439	Pa×s	354.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54478e+01
Coeff. B	-4.62610e+03
Coeff. C	-8.29720e+01
Temperature range (K), min.	354.15
Temperature range (K), max.	539.36

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=C526852&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume