Phenol, 2,3,5-trimethyl-

Other names: 1-Hydroxy-2,3,5-trimethylbenzene
2,3,5-Trimethylphenol
Isopseudocumenol
Inchi: InChI=1S/C9H12O/c1-6-4-7(2)8(3)9(10)5-6/h4-5,10H,1-3H3
InchiKey: OGRAOKJKVGDSFR-UHFFFAOYSA-N
Formula: C9H12O
SMILES: Cc1cc(C)c(C)c(O)c1
Mol. weight [g/mol]: 136.19
CAS: 697-82-5

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
rinpol	1247.00		NIST Webbook
rinpol	217.22		NIST Webbook
rinpol	214.70		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1276.10		NIST Webbook
rinpol	1277.20		NIST Webbook

rinpol	1279.70		NIST Webbook
rinpol	1236.00		NIST Webbook
ripol	2211.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2248.00		NIST Webbook
ripol	2248.00		NIST Webbook
tb	522.58	K	Joback Method
tc	747.15	K	Joback Method
tf	354.37	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.54	J/mol×K	709.72	Joback Method
cpg	329.50	J/mol×K	747.15	Joback Method
cpg	266.77	J/mol×K	522.58	Joback Method
cpg	278.94	J/mol×K	560.01	Joback Method
cpg	290.34	J/mol×K	597.44	Joback Method
cpg	301.03	J/mol×K	634.86	Joback Method
cpg	311.07	J/mol×K	672.29	Joback Method
dvisc	0.0000662	Pa×s	522.58	Joback Method
dvisc	0.0000978	Pa×s	494.54	Joback Method
dvisc	0.0017439	Pa×s	354.37	Joback Method
dvisc	0.0008278	Pa×s	382.40	Joback Method
dvisc	0.0004351	Pa×s	410.44	Joback Method
dvisc	0.0002482	Pa×s	438.47	Joback Method
dvisc	0.0001515	Pa×s	466.51	Joback Method
hvapt	55.10	kJ/mol	442.50	NIST Webbook
hvapt	53.90	kJ/mol	490.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54465e+01

Coeff. B	-4.61306e+03
Coeff. C	-8.25270e+01
Temperature range (K), min.	368.15
Temperature range (K), max.	537.69

Sources

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
Solubilities of Substituted Phenols in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je060058e
Effect of Isomers on Partition Coefficients for Phenolic Compounds in the 1-Butyl-3-methylimidazolium Hexafluorophosphate + Water Two-Phase System:	https://www.doi.org/10.1021/je100016z
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=C697825&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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

Latest version available from: