

Phenol, 3,4,5-trimethyl-

Other names:	1-Hydroxy-3,4,5-trimethylbenzene 3,4,5-Hemimellitenol 3,4,5-Trimethylphenol 5-Hydroxy-1,2,3-trimethylbenzene
Inchi:	InChI=1S/C9H12O/c1-6-4-9(10)5-7(2)8(6)3/h4-5,10H,1-3H3
InchiKey:	FDQQNNZKEJIHMS-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	<chem>Cc1cc(O)cc(C)c1C</chem>
Mol. weight [g/mol]:	136.19
CAS:	527-54-8

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	1346.00		NIST Webbook
rinpol	215.23		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	225.40		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	215.23		NIST Webbook
rinpol	1288.00		NIST Webbook
ripol	2303.00		NIST Webbook
ripol	2303.00		NIST Webbook
tb	521.65 ± 3.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tb	521.65 ± 3.00	K	NIST Webbook
tb	521.70	K	NIST Webbook

tb	524.75 ± 3.00	K	NIST Webbook
tb	521.65 ± 3.00	K	NIST Webbook
tb	525.05 ± 3.00	K	NIST Webbook
tc	747.15	K	Joback Method
tf	381.15 ± 2.00	K	NIST Webbook
tf	380.65 ± 2.00	K	NIST Webbook
tf	378.30 ± 2.00	K	NIST Webbook
tf	382.15 ± 2.00	K	NIST Webbook
tf	379.15 ± 3.00	K	NIST Webbook
tf	379.15 ± 3.00	K	NIST Webbook
tf	382.15 ± 2.00	K	NIST Webbook
tf	382.60 ± 1.00	K	NIST Webbook
tf	380.15 ± 2.00	K	NIST Webbook
tf	382.15 ± 2.00	K	NIST Webbook
vc	0.398	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	320.54	J/mol×K	709.72	Joback Method
cpg	329.50	J/mol×K	747.15	Joback Method
dvisc	0.0017439	Paxs	354.37	Joback Method
dvisc	0.0008278	Paxs	382.40	Joback Method
dvisc	0.0004351	Paxs	410.44	Joback Method
dvisc	0.0002482	Paxs	438.47	Joback Method
dvisc	0.0001515	Paxs	466.51	Joback Method
dvisc	0.0000978	Paxs	494.54	Joback Method
dvisc	0.0000662	Paxs	522.58	Joback Method
hvapt	61.10	kJ/mol	458.50	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54590e+01
Coeff. B	-4.74673e+03
Coeff. C	-8.70860e+01
Temperature range (K), min.	381.15
Temperature range (K), max.	554.86

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C527548&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/ci9903071
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
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

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