5-Isopropyl-3-methylphenol

Other names: 3-isopropyl-5-methyl phenol
Phenol, 3-methyl-5-(1-methylethyl)-
5-isopropyl-m-cresol
Inchi: InChI=1S/C10H14O/c1-7(2)9-4-8(3)5-10(11)6-9/h4-7,11H,1-3H3
InchiKey: ZDUIHRJGDMTBEX-UHFFFAOYSA-N
Formula: C10H14O
SMILES: Cc1cc(O)cc(C(C)C)c1
Mol. weight [g/mol]: 150.22
CAS: 3228-03-3

Physical Properties

Property code	Value	Unit	Source
chs	-5636.00	kJ/mol	NIST Webbook
gf	-20.96	kJ/mol	Joback Method
hf	-210.10	kJ/mol	NIST Webbook
hfs	-300.00	kJ/mol	NIST Webbook
hfus	17.57	kJ/mol	Joback Method
hsub	91.13	kJ/mol	NIST Webbook
hsub	89.90	kJ/mol	NIST Webbook
hvap	53.42	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.824		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
ripol	2287.00		NIST Webbook
ripol	2197.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2197.00		NIST Webbook
ripol	2287.00		NIST Webbook
tb	514.15 ± 4.00	K	NIST Webbook
tb	514.20	K	NIST Webbook
tb	514.15 ± 4.00	K	NIST Webbook
tb	514.15 ± 5.00	K	NIST Webbook
tb	514.15 ± 4.00	K	NIST Webbook
tc	764.51	K	Joback Method
tf	321.65 ± 2.00	K	NIST Webbook
tf	327.15 ± 3.00	K	NIST Webbook

tf	322.65 ± 2.00	K	NIST Webbook
tf	327.15 ± 3.00	K	NIST Webbook
tf	322.55 ± 2.00	K	NIST Webbook
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.65	J/mol×K	540.04	Joback Method
cpg	325.50	J/mol×K	577.45	Joback Method
cpg	338.45	J/mol×K	614.86	Joback Method
cpg	350.56	J/mol×K	652.28	Joback Method
cpg	361.90	J/mol×K	689.69	Joback Method
cpg	372.56	J/mol×K	727.10	Joback Method
cpg	382.61	J/mol×K	764.51	Joback Method
dvisc	0.0035167	Pa×s	338.12	Joback Method
dvisc	0.0012767	Pa×s	371.77	Joback Method
dvisc	0.0005484	Pa×s	405.43	Joback Method
dvisc	0.0002681	Pa×s	439.08	Joback Method
dvisc	0.0001452	Pa×s	472.73	Joback Method
dvisc	0.0000853	Pa×s	506.39	Joback Method
dvisc	0.0000535	Pa×s	540.04	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.70	K	0.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3228033&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume