2-Methyl-6-propylphenol

Other names: Phenol, 2-methyl-6-propyl-
Inchi: InChI=1S/C10H14O/c1-3-5-9-7-4-6-8(2)10(9)11/h4,6-7,11H,3,5H2,1-2H3
InchiKey: NXSQQKKFGJHACS-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCCc1cccc(C)c1O
Mol. weight [g/mol]: 150.22
CAS: 3520-52-3

Physical Properties

Property code	Value	Unit	Source
gf	-18.52	kJ/mol	Joback Method
hf	-201.98	kJ/mol	Joback Method
hfus	21.09	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.653		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
rinpol	1320.00		NIST Webbook
tb	540.48	K	Joback Method
tc	759.98	K	Joback Method
tf	353.12	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.31	J/mol×K	540.48	Joback Method
cpg	370.79	J/mol×K	723.39	Joback Method
cpg	360.34	J/mol×K	686.81	Joback Method
cpg	349.24	J/mol×K	650.23	Joback Method
cpg	337.41	J/mol×K	613.65	Joback Method
cpg	324.79	J/mol×K	577.06	Joback Method
cpg	380.67	J/mol×K	759.98	Joback Method

dvisc	0.0000567	Pa×s	540.48	Joback Method
dvisc	0.0000868	Pa×s	509.25	Joback Method
dvisc	0.0001403	Pa×s	478.03	Joback Method
dvisc	0.0002427	Pa×s	446.80	Joback Method
dvisc	0.0004558	Pa×s	415.57	Joback Method
dvisc	0.0009482	Pa×s	384.35	Joback Method
dvisc	0.0022455	Pa×s	353.12	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59298e+01
Coeff. B	-4.81278e+03
Coeff. C	-8.43200e+01
Temperature range (K), min.	392.00
Temperature range (K), max.	537.57

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3520523&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume