Phenol, 3-(1-methylpropyl)-

Other names: phenol, m-sec-butyl-
Inchi: InChI=1S/C10H14O/c1-3-8(2)9-5-4-6-10(11)7-9/h4-8,11H,3H2,1-2H3
InchiKey: NBYBZLCUXTUWBA-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCC(C)c1cccc(O)c1
Mol. weight [g/mol]: 150.22
CAS: 3522-86-9

Physical Properties

Property code	Value	Unit	Source
gf	-11.33	kJ/mol	Joback Method
hf	-195.79	kJ/mol	Joback Method
hfus	17.96	kJ/mol	Joback Method
hvap	52.76	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.906		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
tb	535.06	K	Joback Method
tc	758.39	K	Joback Method
tf	325.60	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.88	J/mol×K	535.06	Joback Method
cpg	373.98	J/mol×K	721.17	Joback Method
cpg	363.20	J/mol×K	683.95	Joback Method
cpg	351.67	J/mol×K	646.73	Joback Method
cpg	339.34	J/mol×K	609.50	Joback Method
cpg	326.10	J/mol×K	572.28	Joback Method
cpg	384.11	J/mol×K	758.39	Joback Method
dvisc	0.0000572	Pa×s	535.06	Joback Method

dvisc	0.0000944	Pa×s	500.15	Joback Method
dvisc	0.0001678	Pa×s	465.24	Joback Method
dvisc	0.0003276	Pa×s	430.33	Joback Method
dvisc	0.0007197	Pa×s	395.42	Joback Method
dvisc	0.0018414	Pa×s	360.51	Joback Method
dvisc	0.0057625	Pa×s	325.60	Joback Method

Sources

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=C3522869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume