2-(1,1-dimethylpropyl)phenol

Other names: Phenol, 2-(1,1-dimethylpropyl)-
Inchi: InChI=1S/C11H16O/c1-4-11(2,3)9-7-5-6-8-10(9)12/h5-8,12H,4H2,1-3H3
InchiKey: BGRKGHSKCFAPCL-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCC(C)(C)c1ccccc1O
Mol. weight [g/mol]: 164.24
CAS: 3279-27-4

Physical Properties

Property code	Value	Unit	Source
gf	2.37	kJ/mol	Joback Method
hf	-219.90	kJ/mol	Joback Method
hfus	16.66	kJ/mol	Joback Method
hvap	54.07	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	3.080		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	555.15	K	Joback Method
tc	783.63	K	Joback Method
tf	354.29	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.99	J/mol×K	555.15	Joback Method
cpg	376.58	J/mol×K	593.23	Joback Method
cpg	390.98	J/mol×K	631.31	Joback Method
cpg	404.31	J/mol×K	669.39	Joback Method
cpg	416.68	J/mol×K	707.47	Joback Method
cpg	428.20	J/mol×K	745.55	Joback Method
cpg	439.00	J/mol×K	783.63	Joback Method
dvisc	0.0030819	Pa×s	354.29	Joback Method

dvisc	0.0011258	Pa×s	387.77	Joback Method
dvisc	0.0004826	Pa×s	421.24	Joback Method
dvisc	0.0002344	Pa×s	454.72	Joback Method
dvisc	0.0001257	Pa×s	488.20	Joback Method
dvisc	0.0000730	Pa×s	521.67	Joback Method
dvisc	0.0000453	Pa×s	555.15	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=C3279274&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