2-(1,1-Dimethylethyl)-6-(1-methylethyl)phenol

Other names: 2-tert-Butyl-6-isopropylphenol
2-Isopropyl-6-tert-butylphenol
Inchi: InChI=1S/C13H20O/c1-9(2)10-7-6-8-11(12(10)14)13(3,4)5/h6-9,14H,1-5H3
InchiKey: LBLLGKZRDSWOJS-UHFFFAOYSA-N
Formula: C13H20O
SMILES: CC(C)c1cccc(C(C)(C)C)c1O
Mol. weight [g/mol]: 192.30
CAS: 22791-95-3

Physical Properties

Property code	Value	Unit	Source
chl	-7644.00	kJ/mol	NIST Webbook
gf	7.14	kJ/mol	Joback Method
hf	-241.00	kJ/mol	NIST Webbook
hfl	-330.00	kJ/mol	NIST Webbook
hfus	17.92	kJ/mol	Joback Method
hvap	90.17	kJ/mol	NIST Webbook
hvap	89.00	kJ/mol	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.813		Crippen Method
mcvol	176.140	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
rinpol	1382.70		NIST Webbook
rinpol	1382.70		NIST Webbook
tb	605.45	K	Joback Method
tc	831.25	K	Joback Method
tf	374.35	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.90	J/mol×K	605.45	Joback Method
cpg	474.73	J/mol×K	643.08	Joback Method

cpg	490.42	J/mol×K	680.72	Joback Method
cpg	505.07	J/mol×K	718.35	Joback Method
cpg	518.79	J/mol×K	755.98	Joback Method
cpg	531.69	J/mol×K	793.62	Joback Method
cpg	543.89	J/mol×K	831.25	Joback Method
dvisc	0.0019883	Pa×s	374.35	Joback Method
dvisc	0.0006796	Pa×s	412.87	Joback Method
dvisc	0.0002790	Pa×s	451.38	Joback Method
dvisc	0.0001317	Pa×s	489.90	Joback Method
dvisc	0.0000694	Pa×s	528.42	Joback Method
dvisc	0.0000399	Pa×s	566.93	Joback Method
dvisc	0.0000246	Pa×s	605.45	Joback Method

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=C22791953&Units=SI

Legend

chl: Standard liquid 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
hfl: Liquid phase 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume