2-Butyl-4-methyl phenol

Other names: 2-butyl-p-cresol
Inchi: InChI=1S/C11H16O/c1-3-4-5-10-8-9(2)6-7-11(10)12/h6-8,12H,3-5H2,1-2H3
InchiKey: FEXBEKLLSUWSIM-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCCCc1cc(C)ccc1O
Mol. weight [g/mol]: 164.24
CAS: 6891-45-8

Physical Properties

Property code	Value	Unit	Source
gf	-10.10	kJ/mol	Joback Method
hf	-222.62	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.043		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
tb	563.36	K	Joback Method
tc	779.08	K	Joback Method
tf	364.39	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.32	J/mol×K	563.36	Joback Method
cpg	420.72	J/mol×K	743.13	Joback Method
cpg	409.51	J/mol×K	707.17	Joback Method
cpg	397.64	J/mol×K	671.22	Joback Method
cpg	385.03	J/mol×K	635.27	Joback Method
cpg	371.61	J/mol×K	599.31	Joback Method

cpg	431.33	J/mol×K	779.08	Joback Method
dvisc	0.0000453	Pa×s	563.36	Joback Method
dvisc	0.0000695	Pa×s	530.20	Joback Method
dvisc	0.0001126	Pa×s	497.04	Joback Method
dvisc	0.0001957	Pa×s	463.88	Joback Method
dvisc	0.0003702	Pa×s	430.71	Joback Method
dvisc	0.0007789	Pa×s	397.55	Joback Method
dvisc	0.0018765	Pa×s	364.39	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6891458&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

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

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