4-allyl-2,6-dimethyl-phenol

Inchi: InChI=1S/C11H14O/c1-4-5-10-6-8(2)11(12)9(3)7-10/h4,6-7,12H,1,5H2,2-3H3
InchiKey: JSETXDOJYIQIST-UHFFFAOYSA-N
Formula: C11H14O
SMILES: C=CCc1cc(C)c(O)c(C)c1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	68.11	kJ/mol	Joback Method
hf	-108.66	kJ/mol	Joback Method
hfus	22.01	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.738		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	565.02	K	Joback Method
tc	786.43	K	Joback Method
tf	375.15	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.13	J/mol×K	565.02	Joback Method
cpg	396.01	J/mol×K	749.53	Joback Method
cpg	385.61	J/mol×K	712.63	Joback Method
cpg	374.59	J/mol×K	675.73	Joback Method
cpg	362.89	J/mol×K	638.82	Joback Method
cpg	350.43	J/mol×K	601.92	Joback Method
cpg	405.87	J/mol×K	786.43	Joback Method
dvisc	0.0000450	Pa×s	565.02	Joback Method

dvisc	0.0000665	Pa×s	533.38	Joback Method
dvisc	0.0001034	Pa×s	501.73	Joback Method
dvisc	0.0001704	Pa×s	470.08	Joback Method
dvisc	0.0003019	Pa×s	438.44	Joback Method
dvisc	0.0005845	Pa×s	406.79	Joback Method
dvisc	0.0012654	Pa×s	375.15	Joback Method

Sources

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=R279460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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