

2-Allyl-6-t-butylphenol

Inchi:	InChI=1S/C13H18O/c1-5-7-10-8-6-9-11(12(10)14)13(2,3)4/h5-6,8-9,14H,1,7H2,2-4H3
InchiKey:	JHCFLUGYQKACEJ-UHFFFAOYSA-N
Formula:	C13H18O
SMILES:	C=CCc1cccc(C(C)(C)C)c1O
Mol. weight [g/mol]:	190.28
CAS:	3354-55-0

Physical Properties

Property code	Value	Unit	Source
gf	97.42	kJ/mol	Joback Method
hf	-147.22	kJ/mol	Joback Method
hfus	20.17	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.418		Crippen Method
mcvol	171.840	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	602.57	K	Joback Method
tc	828.31	K	Joback Method
tf	387.59	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.38	J/mol×K	602.57	Joback Method
cpg	452.19	J/mol×K	640.19	Joback Method
cpg	466.88	J/mol×K	677.82	Joback Method
cpg	480.57	J/mol×K	715.44	Joback Method
cpg	493.38	J/mol×K	753.07	Joback Method
cpg	505.43	J/mol×K	790.69	Joback Method
cpg	516.82	J/mol×K	828.31	Joback Method
dvisc	0.0013350	Pa×s	387.59	Joback Method
dvisc	0.0005331	Pa×s	423.42	Joback Method

dvisc	0.0002457	Pa×s	459.25	Joback Method
dvisc	0.0001266	Pa×s	495.08	Joback Method
dvisc	0.0000714	Pa×s	530.91	Joback Method
dvisc	0.0000433	Pa×s	566.74	Joback Method
dvisc	0.0000278	Pa×s	602.57	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=C3354550&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

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