

2-ALLYL-6-METHYLPHENOL

Other names:	6-Allyl-o-cresol 6-Allyl-2-cresol 2-Allyl-6-methylphenol 6-Allyl-2-methylphenol o-Cresol, 6-allyl- 2-Methyl-6-(2-propenyl)phenol
Inchi:	InChI=1S/C10H12O/c1-3-5-9-7-4-6-8(2)10(9)11/h3-4,6-7,11H,1,5H2,2H3
InchiKey:	WREVCRYZAWNLRZ-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	C=CCc1cccc(C)c1O
Mol. weight [g/mol]:	148.21

Physical Properties

Property code	Value	Unit	Source
hf	-67.10	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	72.65	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
log10ws	-1.75		Cheméo Relay (1.0)
logp	2.429		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
tb	505.20	K	NIST Webbook
tc	723.23	K	Cheméo Relay (1.0)
tf	287.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.39	J/mol×K	537.16	Joback Method
cpg	357.24	J/mol×K	761.51	Joback Method
cpg	348.11	J/mol×K	724.12	Joback Method
cpg	338.41	J/mol×K	686.73	Joback Method
cpg	328.08	J/mol×K	649.34	Joback Method
cpg	317.01	J/mol×K	611.94	Joback Method

cpg	305.14	J/mol×K	574.55	Joback Method
dvisc	0.0002488	Pa×s	444.26	Joback Method
dvisc	0.0000593	Pa×s	537.16	Joback Method
dvisc	0.0000903	Pa×s	506.19	Joback Method
dvisc	0.0001450	Pa×s	475.23	Joback Method
dvisc	0.0022258	Pa×s	351.36	Joback Method
dvisc	0.0004629	Pa×s	413.29	Joback Method
dvisc	0.0009526	Pa×s	382.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3354583&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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