

Phenol, p-(2-methylallyl)-

Other names:	p(2-methylallyl)-phenol
Inchi:	InChI=1S/C10H12O/c1-8(2)7-9-3-5-10(11)6-4-9/h3-6,11H,1,7H2,2H3
InchiKey:	OVBJIGPDFPHEJT-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	C=C(C)Cc1ccc(O)cc1
Mol. weight [g/mol]:	148.20
CAS:	33641-78-0

Physical Properties

Property code	Value	Unit	Source
gf	70.40	kJ/mol	Joback Method
hf	-74.87	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	52.55	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.511		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
ripol	2277.00		NIST Webbook
tb	532.06	K	Joback Method
tc	759.59	K	Joback Method
tf	324.88	K	Joback Method
vc	0.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.58	J/mol×K	532.06	Joback Method
cpg	305.92	J/mol×K	569.98	Joback Method
cpg	318.26	J/mol×K	607.90	Joback Method
cpg	329.71	J/mol×K	645.82	Joback Method
cpg	340.36	J/mol×K	683.75	Joback Method
cpg	350.29	J/mol×K	721.67	Joback Method
cpg	359.61	J/mol×K	759.59	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=C33641780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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