

Phenol, 4-[1-methyl-1-(1,1-dimethylethyl)butyl]

Inchi:	InChI=1S/C15H24O/c1-6-11-15(5,14(2,3)4)12-7-9-13(16)10-8-12/h7-10,16H,6,11H2,1-5H
InchiKey:	HTBKTFQXEZNFLLH-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CCCC(C)(c1ccc(O)cc1)C(C)(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	38.89	kJ/mol	Joback Method
hf	-311.21	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.496		Crippen Method
mvol	204.320	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1758.00		NIST Webbook
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tb	643.44	K	Joback Method
tc	868.39	K	Joback Method
tf	401.79	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.32	J/molxK	643.44	Joback Method
cpg	643.47	J/molxK	830.89	Joback Method
cpg	629.45	J/molxK	793.40	Joback Method
cpg	614.58	J/molxK	755.91	Joback Method
cpg	598.70	J/molxK	718.42	Joback Method
cpg	581.66	J/molxK	680.93	Joback Method
cpg	656.77	J/molxK	868.39	Joback Method
dvisc	0.0000151	Paxs	643.44	Joback Method

dvisc	0.0000247	Paxs	603.17	Joback Method
dvisc	0.0000434	Paxs	562.89	Joback Method
dvisc	0.0000832	Paxs	522.62	Joback Method
dvisc	0.0001777	Paxs	482.34	Joback Method
dvisc	0.0004357	Paxs	442.07	Joback Method
dvisc	0.0012794	Paxs	401.79	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=R592337&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
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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