

Phenol, 4-[2,3-dimethyl-1-(1-methylethyl)butyl], diastereomer # 1

InChI: InChI=1S/C15H24O/c1-10(2)12(5)15(11(3)4)13-6-8-14(16)9-7-13/h6-12,15-16H,1-5H3
InChIKey: FDNLHRDTAJCZRO-UHFFFAOYSA-N

Formula: C15H24O

SMILES: CC(C)C(C)C(c1ccc(O)cc1)C(C)C

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	23.45	kJ/mol	Joback Method
hf	-314.83	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	4.424		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinqol	1745.00		NIST Webbook
tb	648.14	K	Joback Method
tc	865.70	K	Joback Method
tf	336.95	K	Joback Method
vc	0.710	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.41	J/molxK	648.14	Joback Method
cpg	577.68	J/molxK	684.40	Joback Method
cpg	594.82	J/molxK	720.66	Joback Method
cpg	610.93	J/molxK	756.92	Joback Method
cpg	626.10	J/molxK	793.18	Joback Method
cpg	640.43	J/molxK	829.44	Joback Method
cpg	654.00	J/molxK	865.70	Joback Method
dvisc	0.0079615	Paxs	336.95	Joback Method
dvisc	0.0013836	Paxs	388.81	Joback Method

dvisc	0.0003630	Paxs	440.68	Joback Method
dvisc	0.0001262	Paxs	492.54	Joback Method
dvisc	0.0000537	Paxs	544.41	Joback Method
dvisc	0.0000265	Paxs	596.27	Joback Method
dvisc	0.0000146	Paxs	648.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R592946&Units=SI

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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