

Phenol, 4-(2-methyl-1-(1,1-dimethylethyl)butyl), diastereomer # 1

InChI: InChI=1S/C15H24O/c1-6-11(2)14(15(3,4)5)12-7-9-13(16)10-8-12/h7-11,14,16H,6H2,1-5H
InChIKey: GWBBAZHWDSTSBG-UHFFFAOYSA-N

Formula: C15H24O

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

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	31.17	kJ/mol	Joback Method
hf	-313.02	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1733.00		NIST Webbook
tb	645.79	K	Joback Method
tc	866.98	K	Joback Method
tf	369.37	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.35	J/molxK	645.79	Joback Method
cpg	641.94	J/molxK	830.11	Joback Method
cpg	627.76	J/molxK	793.25	Joback Method
cpg	612.74	J/molxK	756.38	Joback Method
cpg	596.74	J/molxK	719.52	Joback Method
cpg	579.65	J/molxK	682.65	Joback Method
cpg	655.38	J/molxK	866.98	Joback Method
dvisc	0.0000148	Paxs	645.79	Joback Method
dvisc	0.0000256	Paxs	599.72	Joback Method

dvisc	0.0000484	Paxs	553.65	Joback Method
dvisc	0.0001026	Paxs	507.58	Joback Method
dvisc	0.0002529	Paxs	461.51	Joback Method
dvisc	0.0007611	Paxs	415.44	Joback Method
dvisc	0.0030151	Paxs	369.37	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=R593078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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