

Phenol, 4-butoxy-

Other names:	Phenol, p-butoxy- p-Butoxyphenol 4-Butoxyphenol
Inchi:	InChI=1S/C10H14O2/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7,11H,2-3,8H2,1H3
InchiKey:	MBGGFXOXUIDRJD-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CCCCOc1ccc(O)cc1
Mol. weight [g/mol]:	166.22
CAS:	122-94-1

Physical Properties

Property code	Value	Unit	Source
gf	-113.89	kJ/mol	Joback Method
hf	-322.73	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	55.55	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.571		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	557.92	K	Joback Method
tc	773.80	K	Joback Method
tf	362.83	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.47	J/mol×K	557.92	Joback Method
cpg	395.13	J/mol×K	737.82	Joback Method
cpg	384.62	J/mol×K	701.84	Joback Method
cpg	373.45	J/mol×K	665.86	Joback Method
cpg	361.58	J/mol×K	629.88	Joback Method
cpg	348.94	J/mol×K	593.90	Joback Method

cpg	405.05	J/mol×K	773.80	Joback Method
dvisc	0.0000427	Paxs	557.92	Joback Method
dvisc	0.0000659	Paxs	525.41	Joback Method
dvisc	0.0001078	Paxs	492.89	Joback Method
dvisc	0.0001891	Paxs	460.38	Joback Method
dvisc	0.0003612	Paxs	427.86	Joback Method
dvisc	0.0007674	Paxs	395.35	Joback Method
dvisc	0.0018663	Paxs	362.83	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=C122941&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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