

4-n-Butylphenol, isoBOC

Inchi:	InChI=1S/C15H22O3/c1-4-5-6-13-7-9-14(10-8-13)18-15(16)17-11-12(2)3/h7-10,12H,4-6,
InchiKey:	XUOZTIXYGMJADJ-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	CCCCc1ccc(OC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-163.16	kJ/mol	Joback Method
hf	-510.17	kJ/mol	Joback Method
hfus	28.71	kJ/mol	Joback Method
hvap	63.10	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.201		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1794.00		NIST Webbook
tb	672.53	K	Joback Method
tc	872.85	K	Joback Method
tf	377.14	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.48	J/molxK	672.53	Joback Method
cpg	591.05	J/molxK	705.92	Joback Method
cpg	606.69	J/molxK	739.30	Joback Method
cpg	621.42	J/molxK	772.69	Joback Method
cpg	635.24	J/molxK	806.08	Joback Method
cpg	648.16	J/molxK	839.47	Joback Method
cpg	660.21	J/molxK	872.85	Joback Method
dvisc	0.0013204	Paxs	377.14	Joback Method
dvisc	0.0006665	Paxs	426.37	Joback Method

dvisc	0.0003875	Paxs	475.60	Joback Method
dvisc	0.0002495	Paxs	524.84	Joback Method
dvisc	0.0001732	Paxs	574.07	Joback Method
dvisc	0.0001274	Paxs	623.30	Joback Method
dvisc	0.0000980	Paxs	672.53	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=R235222&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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