

4-n-Propylphenol, isoBOC

Inchi:	InChI=1S/C14H20O3/c1-4-5-12-6-8-13(9-7-12)17-14(15)16-10-11(2)3/h6-9,11H,4-5,10H
InchiKey:	ACXYXVROPRAZEU-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCc1ccc(OC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
gf	-171.58	kJ/mol	Joback Method
hf	-489.53	kJ/mol	Joback Method
hfus	26.12	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.810		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	649.65	K	Joback Method
tc	852.56	K	Joback Method
tf	365.87	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.47	J/molxK	649.65	Joback Method
cpg	537.60	J/molxK	683.47	Joback Method
cpg	552.84	J/molxK	717.29	Joback Method
cpg	567.20	J/molxK	751.10	Joback Method
cpg	580.68	J/molxK	784.92	Joback Method
cpg	593.31	J/molxK	818.74	Joback Method
cpg	605.07	J/molxK	852.56	Joback Method
dvisc	0.0014110	Paxs	365.87	Joback Method

dvisc	0.0007226	Paxs	413.17	Joback Method
dvisc	0.0004246	Paxs	460.46	Joback Method
dvisc	0.0002754	Paxs	507.76	Joback Method
dvisc	0.0001924	Paxs	555.06	Joback Method
dvisc	0.0001421	Paxs	602.35	Joback Method
dvisc	0.0001098	Paxs	649.65	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=R235242&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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