2-n-Propylphenol, isoBOC

Inchi: InChI=1S/C14H20O3/c1-4-7-12-8-5-6-9-13(12)17-14(15)16-10-11(2)3/h5-6,8-9,11H,4,7,1
InchiKey: ODHWFJGBUOCREP-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: CCCc1ccccc1OC(=O)OCC(C)C
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	1591.00		NIST Webbook
rinpol	1591.00		NIST Webbook
tb	649.65	K	Joback Method
tc	852.56	K	Joback Method
tf	365.87	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007226	Pa×s	413.17	Joback Method
dvisc	0.0004246	Pa×s	460.46	Joback Method
dvisc	0.0002754	Pa×s	507.76	Joback Method
dvisc	0.0001924	Pa×s	555.06	Joback Method
dvisc	0.0001421	Pa×s	602.35	Joback Method
dvisc	0.0001098	Pa×s	649.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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