

4,5-Dimethoxy-2-(2-propyl)phenol

Inchi:	InChI=1S/C11H16O3/c1-7(2)8-5-10(13-3)11(14-4)6-9(8)12/h5-7,12H,1-4H3
InchiKey:	NRQXZAIQWCSHP-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	COc1cc(O)c(C(C)C)cc1OC
Mol. weight [g/mol]:	196.24

Physical Properties

Property code	Value	Unit	Source
gf	-232.17	kJ/mol	Joback Method
hf	-503.81	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	61.13	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	2.533		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	612.74	K	Joback Method
tc	828.87	K	Joback Method
tf	406.37	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.33	J/molxK	612.74	Joback Method
cpg	468.59	J/molxK	792.85	Joback Method
cpg	457.45	J/molxK	756.83	Joback Method
cpg	445.69	J/molxK	720.81	Joback Method
cpg	433.27	J/molxK	684.78	Joback Method
cpg	420.16	J/molxK	648.76	Joback Method
cpg	479.13	J/molxK	828.87	Joback Method
dvisc	0.0000202	Paxs	612.74	Joback Method

dvisc	0.0000300	Paxs	578.35	Joback Method
dvisc	0.0000469	Paxs	543.95	Joback Method
dvisc	0.0000777	Paxs	509.56	Joback Method
dvisc	0.0001386	Paxs	475.16	Joback Method
dvisc	0.0002705	Paxs	440.76	Joback Method
dvisc	0.0005911	Paxs	406.37	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=R404978&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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