

Benzene, 1-methoxy-4-propyl-

Other names:	Anisole, p-propyl- p-Propylanisole Dihydroanethole 4-n-Propylanisole 4-Propylanisole p-n-Propylanisole 1-Methoxy-4-propylbenzene p-Propylmethoxybenzene Methyl p-propylphenyl ether p-Propylphenol methyl ether NSC 37996 propylanisol
Inchi:	InChI=1S/C10H14O/c1-3-4-9-5-7-10(11-2)8-6-9/h5-8H,3-4H2,1-2H3
InchiKey:	KBHWKXNXTURZCD-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CCc1ccc(OC)cc1
Mol. weight [g/mol]:	150.22
CAS:	104-45-0

Physical Properties

Property code	Value	Unit	Source
gf	31.10	kJ/mol	Joback Method
hf	-156.89	kJ/mol	Joback Method
hfus	16.50	kJ/mol	Joback Method
hvap	43.20	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.648		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
ripol	1606.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1606.00		NIST Webbook
tb	488.50 ± 0.50	K	NIST Webbook
tc	686.66	K	Joback Method
tf	263.63	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.65	J/molxK	482.28	Joback Method
cpg	346.49	J/molxK	652.59	Joback Method
cpg	334.82	J/molxK	618.53	Joback Method
cpg	322.51	J/molxK	584.47	Joback Method
cpg	309.56	J/molxK	550.41	Joback Method
cpg	295.94	J/molxK	516.34	Joback Method
cpg	357.54	J/molxK	686.66	Joback Method
dvisc	0.0001871	Paxs	482.28	Joback Method
dvisc	0.0002355	Paxs	445.84	Joback Method
dvisc	0.0003087	Paxs	409.40	Joback Method
dvisc	0.0004268	Paxs	372.95	Joback Method
dvisc	0.0006327	Paxs	336.51	Joback Method
dvisc	0.0010323	Paxs	300.07	Joback Method
dvisc	0.0019281	Paxs	263.63	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=C104450&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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