

2-Ethyl-5-n-propylphenol

Other names:	2-Ethyl-5-propylphenol
Inchi:	InChI=1S/C11H16O/c1-3-5-9-6-7-10(4-2)11(12)8-9/h6-8,12H,3-5H2,1-2H3
InchiKey:	OSQMMONNVPMEIO-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCc1ccc(CC)c(O)c1
Mol. weight [g/mol]:	164.24
CAS:	72386-20-0

Physical Properties

Property code	Value	Unit	Source
gf	-10.10	kJ/mol	Joback Method
hf	-222.62	kJ/mol	Joback Method
hfus	23.68	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.907		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
tb	563.36	K	Joback Method
tc	779.08	K	Joback Method
tf	364.39	K	Joback Method
vc	0.509	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.32	J/mol×K	563.36	Joback Method
cpg	371.61	J/mol×K	599.31	Joback Method
cpg	385.03	J/mol×K	635.27	Joback Method
cpg	397.64	J/mol×K	671.22	Joback Method
cpg	409.51	J/mol×K	707.17	Joback Method
cpg	420.72	J/mol×K	743.13	Joback Method

cpg	431.33	J/mol×K	779.08	Joback Method
dvisc	0.0018765	Paxs	364.39	Joback Method
dvisc	0.0007789	Paxs	397.55	Joback Method
dvisc	0.0003702	Paxs	430.71	Joback Method
dvisc	0.0001957	Paxs	463.88	Joback Method
dvisc	0.0001126	Paxs	497.04	Joback Method
dvisc	0.0000695	Paxs	530.20	Joback Method
dvisc	0.0000453	Paxs	563.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72386200&Units=SI
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

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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