2-Propylphenol, methyl ether

Inchi: InChI=1S/C10H14O/c1-3-6-9-7-4-5-8-10(9)11-2/h4-5,7-8H,3,6H2,1-2H3
InchiKey: RQUBLQRVLBWBLZ-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCCc1ccccc1OC
Mol. weight [g/mol]: 150.22

Physical Properties

Property code	Value	Unit	Source
af	0.4611		Cheméo Relay (1.0)
gf	31.10	kJ/mol	Joback Method
hf	-138.85	kJ/mol	Cheméo Relay (1.0)
hfus	16.50	kJ/mol	Joback Method
hvap	57.86	kJ/mol	Cheméo Relay (1.0)
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	2.648		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1175.30		NIST Webbook
tb	479.74	K	Cheméo Relay (1.0)
tc	681.98	K	Cheméo Relay (1.0)
tf	247.34	K	Cheméo Relay (1.0)
vc	0.492	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-3.08000e-01
Coeff. B	7.52240e-01
Coeff. C	-3.73360e-04
Coeff. D	5.36000e-08

Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.13959e+01
Coeff. B	1.35629e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	263.63
Temperature range (K), max.	480.86

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333484&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie:	Ionization energy
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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