

P-cresol, 2-propentyl-

Inchi:	InChI=1S/C10H12O/c1-3-4-9-7-8(2)5-6-10(9)11/h3-7,11H,1-2H3/b4-3+
InchiKey:	WPHPAOKIUGOXMM-ONEGZZNKSA-N
Formula:	C10H12O
SMILES:	CC=Cc1cc(C)ccc1O
Mol. weight [g/mol]:	148.20
CAS:	53889-94-4

Physical Properties

Property code	Value	Unit	Source
gf	61.70	kJ/mol	Joback Method
hf	-84.76	kJ/mol	Joback Method
hfus	21.29	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.734		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	544.64	K	Joback Method
tc	774.48	K	Joback Method
tf	348.04	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.40	J/molxK	544.64	Joback Method
cpg	348.34	J/molxK	736.17	Joback Method
cpg	338.64	J/molxK	697.86	Joback Method
cpg	328.29	J/molxK	659.56	Joback Method
cpg	317.20	J/molxK	621.25	Joback Method
cpg	305.27	J/molxK	582.95	Joback Method
cpg	357.50	J/molxK	774.48	Joback Method
dvisc	0.0000466	Paxs	544.64	Joback Method
dvisc	0.0000722	Paxs	511.87	Joback Method

dvisc	0.0001188	Paxs	479.11	Joback Method
dvisc	0.0002101	Paxs	446.34	Joback Method
dvisc	0.0004069	Paxs	413.57	Joback Method
dvisc	0.0008830	Paxs	380.81	Joback Method
dvisc	0.0022167	Paxs	348.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53889944&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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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