

O-cresol, 4-(1-methylhexyl)-

Inchi:	InChI=1S/C14H22O/c1-4-5-6-7-11(2)13-8-9-14(15)12(3)10-13/h8-11,15H,4-7H2,1-3H3
InchiKey:	ZMAWSFRVKHOOJU-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CCCCCC(C)c1ccc(O)c(C)c1
Mol. weight [g/mol]:	206.32
CAS:	42433-61-4

Physical Properties

Property code	Value	Unit	Source
gf	12.72	kJ/mol	Joback Method
hf	-289.82	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	62.32	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.384		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	631.56	K	Joback Method
tc	841.06	K	Joback Method
tf	383.20	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.51	J/molxK	631.56	Joback Method
cpg	522.01	J/molxK	666.48	Joback Method
cpg	537.57	J/molxK	701.39	Joback Method
cpg	552.28	J/molxK	736.31	Joback Method
cpg	566.19	J/molxK	771.23	Joback Method
cpg	579.38	J/molxK	806.14	Joback Method
cpg	591.94	J/molxK	841.06	Joback Method
dvisc	0.0015604	Paxs	383.20	Joback Method
dvisc	0.0005413	Paxs	424.59	Joback Method

dvisc	0.0002266	Paxs	465.99	Joback Method
dvisc	0.0001094	Paxs	507.38	Joback Method
dvisc	0.0000589	Paxs	548.77	Joback Method
dvisc	0.0000346	Paxs	590.17	Joback Method
dvisc	0.0000218	Paxs	631.56	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=C42433614&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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