

4-(2-ethylhexyl)phenol

Inchi: InChI=1S/C14H22O/c1-3-5-6-12(4-2)11-13-7-9-14(15)10-8-13/h7-10,12,15H,3-6,11H2,1-
InchiKey: OKUMHINSMZOUIZ-UHFFFAOYSA-N
Formula: C14H22O
SMILES: CCCCC(CC)Cc1ccc(O)cc1
Mol. weight [g/mol]: 206.32

Physical Properties

Property code	Value	Unit	Source
gf	22.35	kJ/mol	Joback Method
hf	-278.35	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	61.66	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.151		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
tb	626.58	K	Joback Method
tc	835.17	K	Joback Method
tf	370.68	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.85	J/mol×K	626.58	Joback Method
cpg	522.56	J/mol×K	661.35	Joback Method
cpg	538.30	J/mol×K	696.11	Joback Method
cpg	553.13	J/mol×K	730.88	Joback Method
cpg	567.13	J/mol×K	765.64	Joback Method
cpg	580.39	J/mol×K	800.41	Joback Method
cpg	592.98	J/mol×K	835.17	Joback Method
dvisc	0.0023538	Pa×s	370.68	Joback Method

dvisc	0.0007286	Pa×s	413.33	Joback Method
dvisc	0.0002808	Pa×s	455.98	Joback Method
dvisc	0.0001274	Pa×s	498.63	Joback Method
dvisc	0.0000655	Pa×s	541.28	Joback Method
dvisc	0.0000371	Pa×s	583.93	Joback Method
dvisc	0.0000227	Pa×s	626.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R256803&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
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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