4-Nonylphenol

Other names: 4-n-Nonyl phenol
4-n-Nonylphenol
Phenol, 4-nonyl-
Phenol, p-nonyl-
p-Nonylphenol
para Nonyl phenol
Inchi: InChI=1S/C15H24O/c1-2-3-4-5-6-7-8-9-14-10-12-15(16)13-11-14/h10-13,16H,2-9H2,1H3
InchiKey: IGFHQQFPSIBGKE-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCCCCCCCc1ccc(O)cc1
Mol. weight [g/mol]: 220.35
CAS: 104-40-5

Physical Properties

Property code	Value	Unit	Source
gf	33.21	kJ/mol	Joback Method
hf	-293.71	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.685		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	1889.00		NIST Webbook
rinpol	1883.40		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1871.80		NIST Webbook
rinpol	1871.80		NIST Webbook
rinpol	1876.70		NIST Webbook
ripol	2900.00		NIST Webbook
tb	649.90	K	Joback Method
tc	851.69	K	Joback Method
tf	396.95	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.92	J/mol×K	851.69	Joback Method
cpg	557.62	J/mol×K	649.90	Joback Method
cpg	574.41	J/mol×K	683.53	Joback Method
cpg	590.28	J/mol×K	717.16	Joback Method
cpg	605.29	J/mol×K	750.79	Joback Method
cpg	619.51	J/mol×K	784.42	Joback Method
cpg	633.03	J/mol×K	818.05	Joback Method
dvisc	0.0000195	Pa×s	649.90	Joback Method
dvisc	0.0012797	Pa×s	396.95	Joback Method
dvisc	0.0004557	Pa×s	439.11	Joback Method
dvisc	0.0001945	Pa×s	481.27	Joback Method
dvisc	0.0000952	Pa×s	523.42	Joback Method
dvisc	0.0000518	Pa×s	565.58	Joback Method
dvisc	0.0000307	Pa×s	607.74	Joback Method
hvapt	65.00	kJ/mol	541.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C104405&Units=SI
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
KDB: https://www.cheric.org/files/research/kdb/mol/mol891.mol

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

hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume