

Phenol, 4-(1,4-dimethylheptyl)

Inchi:	InChI=1S/C15H24O/c1-4-5-12(2)6-7-13(3)14-8-10-15(16)11-9-14/h8-13,16H,4-7H2,1-3H
InchiKey:	AWTNVUASQNOPTK-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CCCC(C)CCC(C)c1ccc(O)cc1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	28.33	kJ/mol	Joback Method
hf	-304.27	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	63.50	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.712		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinsol	1748.00		NIST Webbook
tb	649.02	K	Joback Method
tc	858.39	K	Joback Method
tf	366.95	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.51	J/molxK	649.02	Joback Method
cpg	576.02	J/molxK	683.91	Joback Method
cpg	592.50	J/molxK	718.81	Joback Method
cpg	608.04	J/molxK	753.70	Joback Method
cpg	622.73	J/molxK	788.60	Joback Method
cpg	636.64	J/molxK	823.49	Joback Method
cpg	649.87	J/molxK	858.39	Joback Method
dvisc	0.0028979	Paxs	366.95	Joback Method
dvisc	0.0007553	Paxs	413.96	Joback Method

dvisc	0.0002590	Paxs	460.97	Joback Method
dvisc	0.0001083	Paxs	507.99	Joback Method
dvisc	0.0000525	Paxs	555.00	Joback Method
dvisc	0.0000285	Paxs	602.01	Joback Method
dvisc	0.0000169	Paxs	649.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R592619&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
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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