

Phenol, 4-(1-ethylheptyl)

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H24O/c1-3-5-6-7-8-13(4-2)14-9-11-15(16)12-10-14/h9-13,16H,3-8H2,1-2H

SHAWKHSYQINGHM-UHFFFAOYSA-N

C15H24O

CCCCCCC(CC)c1ccc(O)cc1

220.35

Physical Properties

Property code	Value	Unit	Source
gf	30.77	kJ/mol	Joback Method
hf	-298.99	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.856		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1795.00		NIST Webbook
tb	649.46	K	Joback Method
tc	854.96	K	Joback Method
tf	381.95	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.07	J/mol×K	649.46	Joback Method
cpg	575.21	J/mol×K	683.71	Joback Method
cpg	591.38	J/mol×K	717.96	Joback Method
cpg	606.65	J/mol×K	752.21	Joback Method
cpg	621.10	J/mol×K	786.46	Joback Method
cpg	634.82	J/mol×K	820.71	Joback Method
cpg	647.87	J/mol×K	854.96	Joback Method
dvisc	0.0018851	Pa×s	381.95	Joback Method
dvisc	0.0005800	Pa×s	426.53	Joback Method

dvisc	0.0002231	Pa×s	471.12	Joback Method
dvisc	0.0001012	Pa×s	515.71	Joback Method
dvisc	0.0000521	Pa×s	560.29	Joback Method
dvisc	0.0000295	Pa×s	604.88	Joback Method
dvisc	0.0000181	Pa×s	649.46	Joback Method

Sources

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=R592822&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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