Phenol, 4-[1-ethyl-2-methyl-1-(1-methylpropyl)propyl]

Inchi: InChI=1S/C16H26O/c1-6-13(5)16(7-2,12(3)4)14-8-10-15(17)11-9-14/h8-13,17H,6-7H2,1-

InchiKey: DDJFQXYNOJOKOE-UHFFFAOYSA-N

Formula: C16H26O

SMILES: CCC(C)C(CC)(c1ccc(O)cc1)C(C)C

Mol. weight [g/mol]: 234.38

Physical Properties

Property code	Value	Unit	Source
gf	39.59	kJ/mol	Joback Method
hf	-333.66	kJ/mol	Joback Method
hfus	22.56	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.742		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1994.77	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	668.67	K	Joback Method
tc	886.06	K	Joback Method
tf	380.64	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.70	J/mol×K	668.67	Joback Method
cpg	633.29	J/mol×K	704.90	Joback Method
cpg	650.70	J/mol×K	741.13	Joback Method
cpg	667.06	J/mol×K	777.36	Joback Method
cpg	682.47	J/mol×K	813.60	Joback Method
cpg	697.05	J/mol×K	849.83	Joback Method
cpg	710.92	J/mol×K	886.06	Joback Method
dvisc	0.0023307	Pa×s	380.64	Joback Method

dvisc	0.0005882	Pa×s	428.64	Joback Method
dvisc	0.0001959	Pa×s	476.65	Joback Method
dvisc	0.0000798	Pa×s	524.65	Joback Method
dvisc	0.0000378	Pa×s	572.66	Joback Method
dvisc	0.0000201	Pa×s	620.67	Joback Method
dvisc	0.0000117	Pa×s	668.67	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=R592748&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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