Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethoxy-

Inchi: InChI=1S/C16H26O2/c1-8-18-11-9-12(15(2,3)4)14(17)13(10-11)16(5,6)7/h9-10,17H,8H2
InchiKey: YQQQXXUABFURLN-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCOc1cc(C(C)(C)C)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 250.38
CAS: 5442-35-3

Physical Properties

Property code	Value	Unit	Source
gf	-76.95	kJ/mol	Joback Method
hf	-487.01	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	67.64	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.386		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	1575.00		NIST Webbook
tb	698.70	K	Joback Method
tc	918.63	K	Joback Method
tf	460.33	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.65	J/mol×K	698.70	Joback Method
cpg	722.49	J/mol×K	881.97	Joback Method
cpg	708.43	J/mol×K	845.32	Joback Method
cpg	693.63	J/mol×K	808.66	Joback Method
cpg	677.97	J/mol×K	772.01	Joback Method
cpg	661.35	J/mol×K	735.35	Joback Method
cpg	735.92	J/mol×K	918.63	Joback Method
dvisc	0.0000076	Pa×s	698.70	Joback Method

dvisc	0.0000115	Pa×s	658.97	Joback Method
dvisc	0.0000185	Pa×s	619.24	Joback Method
dvisc	0.0000317	Pa×s	579.52	Joback Method
dvisc	0.0000587	Pa×s	539.79	Joback Method
dvisc	0.0001202	Pa×s	500.06	Joback Method
dvisc	0.0002782	Pa×s	460.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5442353&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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