Phenol, 4-(1,2-diethyl-3-methylbutyl), diastereomer # 1

Inchi: InChI=1S/C15H24O/c1-5-14(11(3)4)15(6-2)12-7-9-13(16)10-8-12/h7-11,14-16H,5-6H2,1-

InchiKey: WPAUFDMVFFNTJO-UHFFFAOYSA-N

Formula: C15H24O

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

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	25.89	kJ/mol	Joback Method
hf	-309.55	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1757.00		NIST Webbook
tb	648.58	K	Joback Method
tc	861.97	K	Joback Method
tf	351.95	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.96	J/mol×K	648.58	Joback Method
cpg	576.84	J/mol×K	684.14	Joback Method
cpg	593.65	J/mol×K	719.71	Joback Method
cpg	609.47	J/mol×K	755.27	Joback Method
cpg	624.40	J/mol×K	790.84	Joback Method
cpg	638.52	J/mol×K	826.40	Joback Method
cpg	651.91	J/mol×K	861.97	Joback Method
dvisc	0.0046742	Pa×s	351.95	Joback Method
dvisc	0.0010084	Pa×s	401.39	Joback Method

dvisc	0.0003045	Pa×s	450.83	Joback Method
dvisc	0.0001165	Pa×s	500.26	Joback Method
dvisc	0.0000530	Pa×s	549.70	Joback Method
dvisc	0.0000275	Pa×s	599.14	Joback Method
dvisc	0.0000157	Pa×s	648.58	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R592515&Units=SI

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