1,1'-Biphenyl, 3,4-diethyl-

Other names: 3,4-Diethyl-1,1'-biphenyl
Inchi: InChI=1S/C16H18/c1-3-13-10-11-16(12-14(13)4-2)15-8-6-5-7-9-15/h5-12H,3-4H2,1-2H3
InchiKey: ZTLWBQOFTIFRHI-UHFFFAOYSA-N
Formula: C16H18
SMILES: CCc1ccc(-c2ccccc2)cc1CC
Mol. weight [g/mol]: 210.31
CAS: 61141-66-0

Physical Properties

Property code	Value	Unit	Source
gf	289.40	kJ/mol	Joback Method
hf	76.55	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.478		Crippen Method
mcvol	188.780	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1692.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2228.00		NIST Webbook
tb	628.80	K	Joback Method
tc	860.73	K	Joback Method
tf	347.96	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.73	J/mol×K	628.80	Joback Method
cpg	489.89	J/mol×K	667.45	Joback Method
cpg	506.82	J/mol×K	706.11	Joback Method
cpg	522.58	J/mol×K	744.76	Joback Method
cpg	537.22	J/mol×K	783.42	Joback Method

cpg	550.82	J/mol×K	822.07	Joback Method
cpg	563.43	J/mol×K	860.73	Joback Method
dvisc	0.0014473	Pa×s	347.96	Joback Method
dvisc	0.0007888	Pa×s	394.77	Joback Method
dvisc	0.0004889	Pa×s	441.57	Joback Method
dvisc	0.0003321	Pa×s	488.38	Joback Method
dvisc	0.0002414	Pa×s	535.19	Joback Method
dvisc	0.0001847	Pa×s	581.99	Joback Method
dvisc	0.0001471	Pa×s	628.80	Joback Method

Sources

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=C61141660&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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