3-Ethylbiphenyl

Other names: 1,1'-Biphenyl, 3-ethyl-
Biphenyl, 3-ethyl-
Inchi: InChI=1S/C14H14/c1-2-12-7-6-10-14(11-12)13-8-4-3-5-9-13/h3-11H,2H2,1H3
InchiKey: HUXKTWJQSHBZIV-UHFFFAOYSA-N
Formula: C14H14
SMILES: CCc1cccc(-c2ccccc2)c1
Mol. weight [g/mol]: 182.26
CAS: 5668-93-9

Physical Properties

Property code	Value	Unit	Source
gf	282.19	kJ/mol	Joback Method
hf	129.30	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.916		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1621.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2190.00		NIST Webbook
tb	559.11 ± 1.00	K	NIST Webbook
tc	818.72	K	Joback Method
tf	245.58 ± 0.20	K	NIST Webbook
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.14	J/mol×K	578.06	Joback Method

cpg	389.56	J/mol×K	618.17	Joback Method
cpg	405.71	J/mol×K	658.28	Joback Method
cpg	420.65	J/mol×K	698.39	Joback Method
cpg	434.45	J/mol×K	738.50	Joback Method
cpg	447.19	J/mol×K	778.61	Joback Method
cpg	458.94	J/mol×K	818.72	Joback Method
dvisc	0.0019467	Pa×s	312.90	Joback Method
dvisc	0.0010159	Pa×s	357.09	Joback Method
dvisc	0.0006118	Pa×s	401.29	Joback Method
dvisc	0.0004075	Pa×s	445.48	Joback Method
dvisc	0.0002920	Pa×s	489.67	Joback Method
dvisc	0.0002212	Pa×s	533.87	Joback Method
dvisc	0.0001748	Pa×s	578.06	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	1.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5668939&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume