

3,5-Diethylbiphenyl

Inchi:	InChI=1S/C16H18/c1-3-13-10-14(4-2)12-16(11-13)15-8-6-5-7-9-15/h5-12H,3-4H2,1-2H3
InchiKey:	BMZIBWSBUQRYBG-UHFFFAOYSA-N
Formula:	C16H18
SMILES:	CCc1cc(CC)cc(-c2ccccc2)c1
Mol. weight [g/mol]:	210.31
CAS:	111154-99-5

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
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/molxK	628.80	Joback Method
cpg	489.89	J/molxK	667.45	Joback Method
cpg	506.82	J/molxK	706.11	Joback Method
cpg	522.58	J/molxK	744.76	Joback Method
cpg	537.22	J/molxK	783.42	Joback Method
cpg	550.82	J/molxK	822.07	Joback Method
cpg	563.43	J/molxK	860.73	Joback Method
dvisc	0.0014473	Paxs	347.96	Joback Method
dvisc	0.0007888	Paxs	394.77	Joback Method

dvisc	0.0004889	Paxs	441.57	Joback Method
dvisc	0.0003321	Paxs	488.38	Joback Method
dvisc	0.0002414	Paxs	535.19	Joback Method
dvisc	0.0001847	Paxs	581.99	Joback Method
dvisc	0.0001471	Paxs	628.80	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=C111154995&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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