3,5-Diisopropylbiphenyl

Other names: 3,5-Diisopropylbiphenyl
Inchi: InChI=1S/C18H22/c1-13(2)16-10-17(14(3)4)12-18(11-16)15-8-6-5-7-9-15/h5-14H,1-4H3
InchiKey: OZIMNQQPGWZXND-UHFFFAOYSA-N
Formula: C18H22
SMILES: CC(C)c1cc(-c2ccccc2)cc(C(C)C)c1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
af	0.5079		Cheméo Relay (1.0)
gf	301.36	kJ/mol	Joback Method
hf	33.44	kJ/mol	Cheméo Relay (1.0)
hfus	22.63	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-6.83		Cheméo Relay (1.0)
logp	5.600		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
tb	595.18	K	Cheméo Relay (1.0)
tc	818.62	K	Cheméo Relay (1.0)
tf	317.02	K	Cheméo Relay (1.0)
vc	0.803	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.18	J/mol×K	673.68	Joback Method
cpg	597.85	J/mol×K	712.39	Joback Method
cpg	616.14	J/mol×K	751.10	Joback Method
cpg	633.14	J/mol×K	789.80	Joback Method
cpg	648.92	J/mol×K	828.51	Joback Method
cpg	663.54	J/mol×K	867.22	Joback Method
cpg	677.08	J/mol×K	905.93	Joback Method

dvisc	0.0020468	Pa×s	340.50	Joback Method
dvisc	0.0008817	Pa×s	396.03	Joback Method
dvisc	0.0004672	Pa×s	451.56	Joback Method
dvisc	0.0002845	Pa×s	507.09	Joback Method
dvisc	0.0001911	Pa×s	562.62	Joback Method
dvisc	0.0001378	Pa×s	618.15	Joback Method
dvisc	0.0001049	Pa×s	673.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69375117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume