

3,5-Di-tert-butylbiphenyl

Inchi:	InChI=1S/C20H26/c1-19(2,3)17-12-16(15-10-8-7-9-11-15)13-18(14-17)20(4,5)6/h7-14H,1
InchiKey:	PMTYHCGSUNDRDL-UHFFFAOYSA-N
Formula:	C20H26
SMILES:	CC(C)(C)c1cc(-c2ccccc2)cc(C(C)(C)C)c1
Mol. weight [g/mol]:	266.42
CAS:	5723-93-3

Physical Properties

Property code	Value	Unit	Source
gf	328.76	kJ/mol	Joback Method
hf	-23.51	kJ/mol	Joback Method
hfus	20.03	kJ/mol	Joback Method
hvap	63.40	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.949		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	713.86	K	Joback Method
tc	953.95	K	Joback Method
tf	397.88	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.07	J/mol×K	713.86	Joback Method
cpg	712.81	J/mol×K	753.88	Joback Method
cpg	731.98	J/mol×K	793.89	Joback Method
cpg	749.69	J/mol×K	833.91	Joback Method
cpg	766.11	J/mol×K	873.92	Joback Method
cpg	781.38	J/mol×K	913.94	Joback Method
cpg	795.62	J/mol×K	953.95	Joback Method
dvisc	0.0012913	Pa×s	397.88	Joback Method
dvisc	0.0005947	Pa×s	450.54	Joback Method

dvisc	0.0003222	Pa×s	503.21	Joback Method
dvisc	0.0001960	Pa×s	555.87	Joback Method
dvisc	0.0001300	Pa×s	608.53	Joback Method
dvisc	0.0000920	Pa×s	661.20	Joback Method
dvisc	0.0000685	Pa×s	713.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5723933&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

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

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