1,1':3',1'':3'',1''':3''',1''''-Quinquephenyl

Other names:	1,1':3',1'':3'',1'''':3''',1''''-quinquephenyl
	m-Quinquiphenyl
	m-quinquephenyl
Inchi:	InChI=1S/C30H22/c1-3-10-23(11-4-1)25-14-7-16-27(20-25)29-18-9-19-30(22-29)28-17-8
InchiKey:	XQCZQOSQCGDDPQ-UHFFFAOYSA-N
Formula:	C30H22
SMILES:	c1ccc(-c2cccc(-c3cccc(-c4cccc(-c5ccccc5)c4)c3)c2)cc1
Mol. weight [g/mol]:	382.50
CAS:	16716-13-5

Physical Properties

Property code	Value	Unit	Source
gf	734.88	kJ/mol	Joback Method
hf	485.71	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	95.74	kJ/mol	Joback Method
ie	8.45 ± 0.05	eV	NIST Webbook
log10ws	-11.88		Crippen Method
logp	8.355		Crippen Method
mcvol	314.760	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	1034.14	K	Joback Method
tc	1323.15	K	Joback Method
tf	597.52	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.86	J/mol×K	1034.14	Joback Method
cpg	1053.65	J/mol×K	1323.15	Joback Method
cpg	1042.19	J/mol×K	1274.98	Joback Method
cpg	1030.55	J/mol×K	1226.81	Joback Method
cpg	1018.47	J/mol×K	1178.64	Joback Method

cpg	1005.67	J/mol×K	1130.48	Joback Method
cpg	991.89	J/mol×K	1082.31	Joback Method
cps	443.70	J/mol×K	298.15	Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series
dvisc	0.0000317	Pa×s	1034.14	Joback Method
dvisc	0.0000399	Pa×s	961.37	Joback Method
dvisc	0.0000522	Pa×s	888.60	Joback Method
dvisc	0.0000716	Pa×s	815.83	Joback Method
dvisc	0.0001045	Pa×s	743.06	Joback Method
dvisc	0.0001656	Pa×s	670.29	Joback Method
dvisc	0.0002934	Pa×s	597.52	Joback Method

Sources

Isomerization effect on the heat capacities and phase behavior of oligophenyls isomers series:	https://www.doi.org/10.1016/j.jct.2013.03.026
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=C16716135&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
cps:	Solid phase 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