

1,1':3',1'':3'',1''':3''',1'''':3'''',1''''':3'''''',1''''':3''''''',1''''''':3'''''''''

Other names:m-Octiphenyl
m-Octaphenyl

Inchi:InChI=1S/C48H34/c1-3-13-35(14-4-1)37-17-7-19-39(29-37)41-21-9-23-43(31-41)45-25-1

InchiKey:QJOBYJDULSYRSC-UHFFFAOYSA-N

Formula:C48H34

SMILES:c1ccc(-c2cccc(-c3cccc(-c4cccc(-c5cccc(-c6cccc(-c7cccc(-c8cccc8)c7)c6)c5)c4)c3)c2)cc

Mol. weight [g/mol]:610.78

CAS:16716-11-3

Physical Properties

Property code	Value	Unit	Source
gf	1194.78	kJ/mol	Joback Method
hf	789.37	kJ/mol	Joback Method
hfus	70.07	kJ/mol	Joback Method
hvap	144.62	kJ/mol	Joback Method
log10ws	-19.69		Crippen Method
logp	13.356		Crippen Method
mcvol	497.100	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
tb	1540.96	K	Joback Method
tc	1886.60	K	Joback Method
tf	917.20	K	Joback Method
vc	1.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1751.07	J/mol×K	1540.96	Joback Method
cpg	1929.11	J/mol×K	1828.99	Joback Method
cpg	1883.88	J/mol×K	1771.38	Joback Method
cpg	1844.16	J/mol×K	1713.78	Joback Method
cpg	1809.26	J/mol×K	1656.17	Joback Method
cpg	1778.46	J/mol×K	1598.57	Joback Method
cpg	1980.57	J/mol×K	1886.60	Joback Method

dvisc	0.0000028	Pa×s	1540.96	Joback Method
dvisc	0.0000035	Pa×s	1437.00	Joback Method
dvisc	0.0000046	Pa×s	1333.04	Joback Method
dvisc	0.0000062	Pa×s	1229.08	Joback Method
dvisc	0.0000089	Pa×s	1125.12	Joback Method
dvisc	0.0000137	Pa×s	1021.16	Joback Method
dvisc	0.0000234	Pa×s	917.20	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=C16716113&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
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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