

1-12-Dodecahydrotetraphenylene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C24H32/c1-2-10-18-17(9-1)19-11-3-4-13-21(19)23-15-7-8-16-24(23)22-14-6-5

AIOOSUVIFSIXAH-LEYBOLSUSA-N

C24H32

C1CCC2=C(C1)C1=C(CCCC1)C1=C(CCCC1)C1=C2CCCC1

320.51

Physical Properties

Property code	Value	Unit	Source
gf	427.40	kJ/mol	Joback Method
hf	10.93	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.482		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	386.36		NIST Webbook
rinpol	386.36		NIST Webbook
tb	880.48	K	Joback Method
tc	1138.31	K	Joback Method
tf	542.66	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.24	J/mol×K	880.48	Joback Method
cpg	952.70	J/mol×K	923.45	Joback Method
cpg	973.77	J/mol×K	966.42	Joback Method
cpg	993.65	J/mol×K	1009.39	Joback Method
cpg	1012.56	J/mol×K	1052.36	Joback Method
cpg	1030.73	J/mol×K	1095.33	Joback Method
cpg	1048.38	J/mol×K	1138.31	Joback Method
dvisc	0.0014143	Pa×s	542.66	Joback Method

dvisc	0.0009403	Pa×s	598.96	Joback Method
dvisc	0.0006705	Pa×s	655.27	Joback Method
dvisc	0.0005045	Pa×s	711.57	Joback Method
dvisc	0.0003957	Pa×s	767.87	Joback Method
dvisc	0.0003208	Pa×s	824.18	Joback Method
dvisc	0.0002672	Pa×s	880.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R214349&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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