

5H-dibenzo[a,d]cycloheptatriene

Other names:	1,2:5,6-Dibenzcycloheptatriene 1,2:5,6-Dibenzotropilidene 2,3:6,7-Dibenzo-4-suberene 2,3:6,7-Dibenzocycloheptatriene 5H-Dibenzo[a,d]cycloheptatriene Dibenzo[a,d]cycloheptatriene Dibenzo[a,d]cycloheptene Dibenzo[a,e]cycloheptatriene Suberene
Inchi:	InChI=1S/C15H12/c1-3-7-14-11-15-8-4-2-6-13(15)10-9-12(14)5-1/h1-10H,11H2
InchiKey:	QPJORFLSOJAUNL-UHFFFAOYSA-N
Formula:	C15H12
SMILES:	C1=Cc2ccccc2Cc2ccccc21
Mol. weight [g/mol]:	192.26

Physical Properties

Property code	Value	Unit	Source
af	0.4011		Cheméo Relay (1.0)
hf	310.97	kJ/mol	Cheméo Relay (1.0)
hfus	20.20	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Cheméo Relay (1.0)
ie	7.77	eV	Cheméo Relay (1.0)
log10ws	-5.38		Cheméo Relay (1.0)
logp	3.761		Crippen Method
mcvol	159.530	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	613.60	K	Cheméo Relay (1.0)
tc	860.95	K	Cheméo Relay (1.0)
tf	400.69	K	Cheméo Relay (1.0)
vc	0.588	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	383.27	J/mol×K	616.49	Joback Method
cpg	463.71	J/mol×K	873.57	Joback Method
cpg	452.94	J/mol×K	830.72	Joback Method
cpg	441.30	J/mol×K	787.87	Joback Method
cpg	428.65	J/mol×K	745.03	Joback Method
cpg	414.86	J/mol×K	702.18	Joback Method
cpg	399.78	J/mol×K	659.34	Joback Method
dvisc	0.0006101	Pa×s	488.06	Joback Method
dvisc	0.0003468	Pa×s	616.49	Joback Method
dvisc	0.0004071	Pa×s	573.68	Joback Method
dvisc	0.0004903	Pa×s	530.87	Joback Method
dvisc	0.0016065	Pa×s	359.63	Joback Method
dvisc	0.0007918	Pa×s	445.25	Joback Method
dvisc	0.0010862	Pa×s	402.44	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C256815&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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