

1,3,5-Cycloheptatriene-7-(2,4,6-cycloheptatrien-1-

Inchi:	InChI=1S/C14H12/c1-2-6-10-13(9-5-1)14-11-7-3-4-8-12-14/h1-12H
InchiKey:	CJRANKZVJIECNW-UHFFFAOYSA-N
Formula:	C14H12
SMILES:	<chem>C1=CC=CC(=C2C=CC=CC=C2)C=C1</chem>
Mol. weight [g/mol]:	180.25
CAS:	531-45-3

Physical Properties

Property code	Value	Unit	Source
gf	297.58	kJ/mol	Joback Method
hf	186.23	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	51.95	kJ/mol	Joback Method
ie	7.00 ± 0.10	eV	NIST Webbook
log10ws	-4.45		Crippen Method
logp	3.647		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	580.78	K	Joback Method
tc	841.19	K	Joback Method
tf	395.00 ± 2.00	K	NIST Webbook
vc	0.574	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.44	J/mol×K	580.78	Joback Method
cpg	373.01	J/mol×K	624.18	Joback Method
cpg	390.04	J/mol×K	667.58	Joback Method
cpg	405.58	J/mol×K	710.99	Joback Method
cpg	419.72	J/mol×K	754.39	Joback Method
cpg	432.53	J/mol×K	797.79	Joback Method
cpg	444.08	J/mol×K	841.19	Joback Method
dvisc	0.0032891	Paxs	294.10	Joback Method

dvisc	0.0012556	Paxs	341.88	Joback Method
dvisc	0.0006070	Paxs	389.66	Joback Method
dvisc	0.0003439	Paxs	437.44	Joback Method
dvisc	0.0002180	Paxs	485.22	Joback Method
dvisc	0.0001499	Paxs	533.00	Joback Method
dvisc	0.0001096	Paxs	580.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C531453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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