

1,4,7,10-Cyclododecatetraene

Inchi:	InChI=1S/C12H16/c1-2-4-6-8-10-12-11-9-7-5-3-1/h1-2,5-8,11-12H,3-4,9-10H2/b2-1-,7-5-
InchiKey:	MHLZRKODFDGPLR-TUVOJHACSA-N
Formula:	C12H16
SMILES:	C1=CCC=CCC=CCC=CC1
Mol. weight [g/mol]:	160.26

Physical Properties

Property code	Value	Unit	Source
gf	129.56	kJ/mol	Joback Method
hf	-22.19	kJ/mol	Joback Method
hfus	9.89	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.785		Crippen Method
mcvol	151.880	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	520.44	K	Joback Method
tc	771.30	K	Joback Method
tf	218.54	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.72	J/molxK	520.44	Joback Method
cpg	352.49	J/molxK	562.25	Joback Method
cpg	373.78	J/molxK	604.06	Joback Method
cpg	393.58	J/molxK	645.87	Joback Method
cpg	411.91	J/molxK	687.68	Joback Method
cpg	428.76	J/molxK	729.49	Joback Method
cpg	444.13	J/molxK	771.30	Joback Method
dvisc	0.0792606	Paxs	218.54	Joback Method
dvisc	0.0077867	Paxs	268.86	Joback Method
dvisc	0.0015899	Paxs	319.17	Joback Method

dvisc	0.0005004	Paxs	369.49	Joback Method
dvisc	0.0002078	Paxs	419.81	Joback Method
dvisc	0.0001041	Paxs	470.12	Joback Method
dvisc	0.0000596	Paxs	520.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U155373&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
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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