

Tricyclo[4.4.2.0(1,6)]dodeca-2,4-diene

Inchi:	InChI=1S/C12H16/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-2,5-6H,3-4,7-10H2
InchiKey:	HAQWKXYXEKTGMS-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	<chem>C1=CC23CCCCC2(C=C1)CC3</chem>
Mol. weight [g/mol]:	160.26
CAS:	33930-87-9

Physical Properties

Property code	Value	Unit	Source
gf	252.76	kJ/mol	Joback Method
hf	157.40	kJ/mol	NIST Webbook
hfus	3.72	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.453		Crippen Method
mcvol	138.760	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	510.46	K	Joback Method
tc	760.27	K	Joback Method
tf	321.82	K	Joback Method
vc	0.523	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.36	J/mol×K	510.46	Joback Method
cpg	355.33	J/mol×K	552.10	Joback Method
cpg	374.10	J/mol×K	593.73	Joback Method
cpg	391.10	J/mol×K	635.37	Joback Method
cpg	406.73	J/mol×K	677.00	Joback Method
cpg	421.43	J/mol×K	718.64	Joback Method
cpg	435.61	J/mol×K	760.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33930879&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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