

Tricyclo[5.3.1.0]undeca-2,4,9-triene

Inchi:	InChI=1S/C11H12/c1-2-5-10-7-4-8-11(10,9-10)6-3-1/h1-5,7H,6,8-9H2
InchiKey:	JZOWWMRTKMEQIK-UHFFFAOYSA-N
Formula:	C11H12
SMILES:	C1=CCC23CC=CC2(C=C1)C3
Mol. weight [g/mol]:	144.21
CAS:	67313-66-0

Physical Properties

Property code	Value	Unit	Source
gf	286.40	kJ/mol	Joback Method
hf	159.87	kJ/mol	Joback Method
hfus	4.45	kJ/mol	Joback Method
hvap	39.05	kJ/mol	Joback Method
ie	7.70	eV	NIST Webbook
log10ws	-3.19		Crippen Method
logp	2.839		Crippen Method
mcvol	120.370	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	482.47	K	Joback Method
tc	730.06	K	Joback Method
tf	314.83	K	Joback Method
vc	0.462	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.71	J/mol×K	482.47	Joback Method
cpg	289.93	J/mol×K	523.74	Joback Method
cpg	305.90	J/mol×K	565.00	Joback Method
cpg	320.04	J/mol×K	606.27	Joback Method
cpg	332.75	J/mol×K	647.53	Joback Method
cpg	344.47	J/mol×K	688.80	Joback Method
cpg	355.61	J/mol×K	730.06	Joback Method

Sources

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=C67313660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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