

Tricyclo[6.1.0.03,5]non-6-ene(1 «alpha»,3 «alpha»,5 «alpha»)

Inchi:	InChI=1S/C9H12/c1-2-7-4-9(7)5-8-3-6(1)8/h1-2,6-9H,3-5H2/t6-,7+,8-,9+
InchiKey:	XFDLCDUCEAMREM-SPJNRGJMSA-N
Formula:	C9H12
SMILES:	C1=CC2CC2CC2CC12
Mol. weight [g/mol]:	120.19
CAS:	62211-22-7

Physical Properties

Property code	Value	Unit	Source
gf	229.40	kJ/mol	Joback Method
hf	26.75	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	35.35	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	2.219		Crippen Method
mcvol	100.790	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	420.03	K	Joback Method
tc	629.91	K	Joback Method
tf	241.53	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.61	J/molxK	420.03	Joback Method
cpg	232.64	J/molxK	455.01	Joback Method
cpg	249.32	J/molxK	489.99	Joback Method
cpg	264.74	J/molxK	524.97	Joback Method
cpg	278.99	J/molxK	559.95	Joback Method
cpg	292.17	J/molxK	594.93	Joback Method
cpg	304.38	J/molxK	629.91	Joback Method
dvisc	0.0002633	Paxs	241.53	Joback Method

dvisc	0.0003673	Paxs	271.28	Joback Method
dvisc	0.0004798	Paxs	301.03	Joback Method
dvisc	0.0005973	Paxs	330.78	Joback Method
dvisc	0.0007171	Paxs	360.53	Joback Method
dvisc	0.0008374	Paxs	390.28	Joback Method
dvisc	0.0009565	Paxs	420.03	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=C62211227&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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