

Tricyclo[6.1.0.0]nonane-(1 «alpha»,2«alpha»,4«alp

Inchi:	InChI=1S/C9H14/c1-2-6-4-8(6)9-5-7(9)3-1/h6-9H,1-5H2/t6-,7+,8+,9-
InchiKey:	UUVWYZVMXOZWNF-OJOKCITNSA-N
Formula:	C9H14
SMILES:	C1CC2CC2C2CC2C1
Mol. weight [g/mol]:	122.21
CAS:	81969-71-3

Physical Properties

Property code	Value	Unit	Source
gf	199.44	kJ/mol	Joback Method
hf	-31.03	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	35.06	kJ/mol	Joback Method
ie	8.95	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	2.442		Crippen Method
mcvol	105.090	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	420.87	K	Joback Method
tc	628.56	K	Joback Method
tf	240.77	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.29	J/molxK	420.87	Joback Method
cpg	311.92	J/molxK	593.94	Joback Method
cpg	297.57	J/molxK	559.33	Joback Method
cpg	282.12	J/molxK	524.71	Joback Method
cpg	265.48	J/molxK	490.10	Joback Method
cpg	247.57	J/molxK	455.48	Joback Method
cpg	325.27	J/molxK	628.56	Joback Method

dvisc	0.0010113	Paxs	420.87	Joback Method
dvisc	0.0009002	Paxs	390.85	Joback Method
dvisc	0.0007860	Paxs	360.84	Joback Method
dvisc	0.0006696	Paxs	330.82	Joback Method
dvisc	0.0005525	Paxs	300.80	Joback Method
dvisc	0.0004369	Paxs	270.79	Joback Method
dvisc	0.0003258	Paxs	240.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81969713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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