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/mol×K	420.87	Joback Method
cpg	311.92	J/mol×K	593.94	Joback Method
cpg	297.57	J/mol×K	559.33	Joback Method
cpg	282.12	J/mol×K	524.71	Joback Method
cpg	265.48	J/mol×K	490.10	Joback Method
cpg	247.57	J/mol×K	455.48	Joback Method
cpg	325.27	J/mol×K	628.56	Joback Method

dvisc	0.0010113	Pa×s	420.87	Joback Method
dvisc	0.0009002	Pa×s	390.85	Joback Method
dvisc	0.0007860	Pa×s	360.84	Joback Method
dvisc	0.0006696	Pa×s	330.82	Joback Method
dvisc	0.0005525	Pa×s	300.80	Joback Method
dvisc	0.0004369	Pa×s	270.79	Joback Method
dvisc	0.0003258	Pa×s	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/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
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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