Tricyclo[4.2.1.02,5]non-7-ene,exo-

Inchi: InChI=1S/C13H20/c1-10-5-6-11(2,9-10)13(4)8-7-12(10,13)3/h5-6H,7-9H2,1-4H3/t10-,11+
InchiKey: AHMLVPKGCGGWRH-FNFFVJSTSA-N
Formula: C9H12
SMILES: CC12C=CC(C)(C1)C1(C)CCC21C
Mol. weight [g/mol]: 120.19
CAS: 16529-82-1

Physical Properties

Property code	Value	Unit	Source
gf	241.12	kJ/mol	Joback Method
hf	5.15	kJ/mol	Joback Method
hfus	0.93	kJ/mol	Joback Method
hvap	39.65	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-3.84		Crippen Method
logp	3.779		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	2790.61	kPa	Joback Method
tb	512.51	K	Joback Method
tc	748.07	K	Joback Method
tf	382.21	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.12	J/mol×K	512.51	Joback Method
cpg	419.50	J/mol×K	551.77	Joback Method
cpg	437.60	J/mol×K	591.03	Joback Method
cpg	454.00	J/mol×K	630.29	Joback Method
cpg	469.27	J/mol×K	669.55	Joback Method
cpg	484.01	J/mol×K	708.81	Joback Method
cpg	498.80	J/mol×K	748.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16529821&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
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