Tricyclo[4.2.1.02,5]non-3-ene

Other names: Tricyclo[4.2.1.0(2,5)]non-7-ene
Inchi: InChI=1S/C9H12/c1-2-7-5-6(1)8-3-4-9(7)8/h1-2,6-9H,3-5H2
InchiKey: XSKXEKKIOLQKBQ-UHFFFAOYSA-N
Formula: C9H12
SMILES: C1=CC2CC1C1CCC21
Mol. weight [g/mol]: 120.19
CAS: 7078-40-2

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/mol×K	420.03	Joback Method
cpg	232.64	J/mol×K	455.01	Joback Method
cpg	249.32	J/mol×K	489.99	Joback Method
cpg	264.74	J/mol×K	524.97	Joback Method
cpg	278.99	J/mol×K	559.95	Joback Method
cpg	292.17	J/mol×K	594.93	Joback Method
cpg	304.38	J/mol×K	629.91	Joback Method

dvisc	0.0002633	Pa×s	241.53	Joback Method
dvisc	0.0003673	Pa×s	271.28	Joback Method
dvisc	0.0004798	Pa×s	301.03	Joback Method
dvisc	0.0005973	Pa×s	330.78	Joback Method
dvisc	0.0007171	Pa×s	360.53	Joback Method
dvisc	0.0008374	Pa×s	390.28	Joback Method
dvisc	0.0009565	Pa×s	420.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7078402&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