

Tricyclo[4.2.1.0(2,5)]non-2(5)-ene

Inchi: InChI=1S/C9H10/c1-2-7-6(1)8-3-4-9(7,8)5-8/h1-5H2
InchiKey: RSXOZYQTOYIEGJ-UHFFFAOYSA-N
Formula: C9H10
SMILES: C1CC2=C1C13CCC21C3
Mol. weight [g/mol]: 118.18
CAS: 41487-78-9

Physical Properties

Property code	Value	Unit	Source
gf	319.34	kJ/mol	Joback Method
hf	240.00	kJ/mol	NIST Webbook
hfus	3.61	kJ/mol	Joback Method
hvap	34.70	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.261		Crippen Method
mcvol	89.930	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
tb	438.41	K	Joback Method
tc	663.87	K	Joback Method
tf	355.59	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.68	J/molxK	438.41	Joback Method
cpg	221.70	J/molxK	475.99	Joback Method
cpg	234.42	J/molxK	513.56	Joback Method
cpg	245.20	J/molxK	551.14	Joback Method
cpg	254.44	J/molxK	588.72	Joback Method
cpg	262.52	J/molxK	626.29	Joback Method
cpg	269.80	J/molxK	663.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41487789&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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