

Bicyclo[2.2.1]hept-2-ene, 2,3-dimethyl-

Other names:	2-Norbornene, 2,3-dimethyl- Santen Santene
Inchi:	InChI=1S/C9H14/c1-6-7(2)9-4-3-8(6)5-9/h8-9H,3-5H2,1-2H3
InchiKey:	LSIXBBPOJBJQHN-UHFFFAOYSA-N
Formula:	C9H14
SMILES:	CC1=C(C)C2CCC1C2
Mol. weight [g/mol]:	122.21
CAS:	529-16-8

Physical Properties

Property code	Value	Unit	Source
gf	145.00	kJ/mol	Joback Method
hf	-54.81	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	37.24	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.753		Crippen Method
mcvol	111.650	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	883.00		NIST Webbook
rinpol	891.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	885.30		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	883.00		NIST Webbook
rinpol	883.00		NIST Webbook
ripol	984.00		NIST Webbook

ripol	991.00		NIST Webbook
ripol	1000.00		NIST Webbook
ripol	1018.00		NIST Webbook
ripol	984.00		NIST Webbook
ripol	997.00		NIST Webbook
tb	432.19	K	Joback Method
tc	636.56	K	Joback Method
tf	249.35	K	Joback Method
vc	0.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.81	J/molxK	432.19	Joback Method
cpg	247.76	J/molxK	466.25	Joback Method
cpg	262.76	J/molxK	500.31	Joback Method
cpg	276.87	J/molxK	534.38	Joback Method
cpg	290.14	J/molxK	568.44	Joback Method
cpg	302.62	J/molxK	602.50	Joback Method
cpg	314.36	J/molxK	636.56	Joback Method
dvisc	0.0006519	Paxs	249.35	Joback Method
dvisc	0.0006129	Paxs	279.82	Joback Method
dvisc	0.0005832	Paxs	310.30	Joback Method
dvisc	0.0005600	Paxs	340.77	Joback Method
dvisc	0.0005412	Paxs	371.24	Joback Method
dvisc	0.0005258	Paxs	401.72	Joback Method
dvisc	0.0005129	Paxs	432.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529168&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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