Bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-

Other names:	2-Bornene
	Bornylene
	1,7,7-Trimethyl-2-norbornene
	1,7,7-Trimethylbicyclo[2.2.1]hept-2-ene
	1,7,7-Trimethylnorbornene
	1,7,7-Trimethyl-bicyclo[2.2.1]hepten-2-ene
	bornylene (2-bornene)
Inchi:	InChI=1S/C10H16/c1-9(2)8-4-6-10(9,3)7-5-8/h4,6,8H,5,7H2,1-3H3
InchiKey:	KUKRLSJNTMLPPK-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	CC12C=CC(CC1)C2(C)C
Mol. weight [g/mol]:	136.23
CAS:	464-17-5

Physical Properties

Property code	Value	Unit	Source
gf	153.99	kJ/mol	Joback Method
hf	-42.37	kJ/mol	Joback Method
hfus	5.52	kJ/mol	Joback Method
hvap	35.53	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.999		Crippen Method
mcvol	125.740	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	907.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	908.90		NIST Webbook
tb	440.92	K	Joback Method
tc	658.12	K	Joback Method
tf	279.14	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.54	J/mol×K	440.92	Joback Method
cpg	292.70	J/mol×K	477.12	Joback Method
cpg	310.04	J/mol×K	513.32	Joback Method
cpg	325.79	J/mol×K	549.52	Joback Method
cpg	340.20	J/mol×K	585.72	Joback Method
cpg	353.50	J/mol×K	621.92	Joback Method
cpg	365.95	J/mol×K	658.12	Joback Method

Sources

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=C464175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume