

Bicyclo[2.2.1]heptane, 2-ethylidene-1,7,7-trimethyl-, (E)-

Other names:	(2E)-2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane 2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane, (E)- (E)-2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane 2-Ethylidene-1,7,7-trimethylbicyclo[2.2.1]heptane
Inchi:	InChI=1S/C12H20/c1-5-9-8-10-6-7-12(9,4)11(10,2)3/h5,10H,6-8H2,1-4H3/b9-5+
InchiKey:	CXSZQFQLQRAPTP-WEVVVXLNSA-N
Formula:	C12H20
SMILES:	CC=C1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	164.29
CAS:	62413-60-9

Physical Properties

Property code	Value	Unit	Source
gf	186.33	kJ/mol	Joback Method
hf	-65.40	kJ/mol	Joback Method
hfus	9.80	kJ/mol	Joback Method
hvap	40.48	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.779		Crippen Method
mcvol	153.920	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	494.16	K	Joback Method
tc	710.52	K	Joback Method
tf	311.28	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.34	J/molxK	494.16	Joback Method
cpg	386.17	J/molxK	530.22	Joback Method
cpg	404.39	J/molxK	566.28	Joback Method
cpg	421.25	J/molxK	602.34	Joback Method
cpg	436.99	J/molxK	638.40	Joback Method

cpg	451.85	J/mol×K	674.46	Joback Method
cpg	466.07	J/mol×K	710.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62413609&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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