3,3-Dimethylbicylo[3.2.0]hepta-1,4-diene

Inchi: InChI=1S/C9H12/c1-9(2)5-7-3-4-8(7)6-9/h5-6H,3-4H2,1-2H3
InchiKey: LCUWWPJEBQOEQH-UHFFFAOYSA-N
Formula: C9H12
SMILES: CC1(C)C=C2CCC2=C1
Mol. weight [g/mol]: 120.19
CAS: 111869-26-2

Physical Properties

Property code	Value	Unit	Source
gf	177.18	kJ/mol	Joback Method
hf	236.00	kJ/mol	NIST Webbook
hfus	7.53	kJ/mol	Joback Method
hvap	36.69	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.673		Crippen Method
mcvol	107.350	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	436.26	K	Joback Method
tc	652.59	K	Joback Method
tf	278.25	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.04	J/mol×K	436.26	Joback Method
cpg	232.76	J/mol×K	472.32	Joback Method
cpg	246.15	J/mol×K	508.37	Joback Method
cpg	258.38	J/mol×K	544.43	Joback Method
cpg	269.59	J/mol×K	580.48	Joback Method
cpg	279.93	J/mol×K	616.54	Joback Method
cpg	289.57	J/mol×K	652.59	Joback Method

Sources

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=C111869262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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