Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-

Other names:	Pinane
	Dihydropinene
	2,6,6-Trimethylbicyclo(3.1.1)heptane
	1a,2b,5a-2,6,6-Trimethylbicyclo(3.1.1)heptane
Inchi:	InChI=1S/C10H18/c1-7-4-5-8-6-9(7)10(8,2)3/h7-9H,4-6H2,1-3H3
InchiKey:	XOKSLPVRUOBDEW-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC1CCC2CC1C2(C)C
Mol. weight [g/mol]:	138.25
CAS:	473-55-2

Physical Properties

Property code	Value	Unit	Source
chl	-6332.90	kJ/mol	NIST Webbook
gf	121.81	kJ/mol	Joback Method
hf	-135.73	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	36.08	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1002.00		NIST Webbook
ripol	1129.00		NIST Webbook
tb	440.90 ± 2.00	K	NIST Webbook
tb	438.00 ± 4.00	K	NIST Webbook
tb	441.75 ± 0.30	K	NIST Webbook
tc	642.10	K	Joback Method
tf	193.05 ± 0.30	K	NIST Webbook
tf	220.00 ± 1.00	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.02	J/mol×K	436.85	Joback Method
cpg	307.28	J/mol×K	471.06	Joback Method
cpg	326.14	J/mol×K	505.27	Joback Method
cpg	343.70	J/mol×K	539.47	Joback Method
cpg	360.10	J/mol×K	573.68	Joback Method
cpg	375.46	J/mol×K	607.89	Joback Method
cpg	389.91	J/mol×K	642.10	Joback Method
cpl	231.80	J/mol×K	313.00	NIST Webbook
cpl	231.40	J/mol×K	311.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C473552&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
cpl: Liquid phase 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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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