Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, (1«alpha»,2«beta»,5«alpha»)-

Other names: 2,6,6-Trimethyl-bicyclo[3.1.1]heptane, cis
2,6,6-Trimethylbicyclo[3.1.1]heptane, (1«alpha»,2«beta»,5«alpha»)-
Pinane, cis
cis-Pinane
(1«alpha»,2«beta»,5«alpha»)-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/t7-,8-,9+/m0/s1

InchiKey: XOKSLPVRUOBDEW-XHNCKOQMSA-N

Formula: C10H18

SMILES: CC1CCC2CC1C2(C)C

Mol. weight [g/mol]: 138.25

CAS: 6876-13-7

Physical Properties

Property code	Value	Unit	Source
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	968.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1075.00		NIST Webbook
ripol	1082.00		NIST Webbook
ripol	1103.00		NIST Webbook
tb	442.00 ± 2.00	K	NIST Webbook

tc	642.10	K	Joback Method
tf	250.24	K	Joback Method
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

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=C6876137&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
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