cis-Pinane

Other names:	(1«alpha»,2«beta»,5«alpha»)-2,6,6-trimethylbicyclo[3.1.1]heptane 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
Inchi:	InChI=1S/C10H18/c1-7-4-5-8-6-9(7)10(8,2)3/h7-9H,4-6H2,1-3H3
InchiKey:	XOKSLPVRUOBDEW-XHNCKOQMSA-N
Formula:	C10H18
SMILES:	CC1CCC2CC1C2(C)C
Mol. weight [g/mol]:	138.25

Physical Properties

Property code	Value	Unit	Source
hf	-70.14	kJ/mol	Cheméo Relay (1.0)
hfus	11.67	kJ/mol	Joback Method
logp	3.079		Crippen Method
mcvol	130.040	ml/mol	McGowan Method
tb	440.21	K	Cheméo Relay (1.0)
tf	252.31	K	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C4755333
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point