

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

Other names:	[1S-(1«alpha»,2«beta»,5«alpha»)]-2,6,6-trimethylbicyclo[3.1.1]heptane cis 2,6,6-trimethylbicyclo[3.1.1]heptane (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-UHFFFAOYSA-N
Formula:	C10H18
SMILES:	CC1CCC2CC1C2(C)C
Mol. weight [g/mol]:	138.25
CAS:	4755-33-3

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
mvol	130.040	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	436.85	K	Joback Method
tc	642.10	K	Joback Method
tf	250.24	K	Joback Method
vc	0.497	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.02	J/molxK	436.85	Joback Method
cpg	307.28	J/molxK	471.06	Joback Method
cpg	326.14	J/molxK	505.27	Joback Method
cpg	343.70	J/molxK	539.47	Joback Method
cpg	360.10	J/molxK	573.68	Joback Method
cpg	375.46	J/molxK	607.89	Joback Method
cpg	389.91	J/molxK	642.10	Joback Method

Sources

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=C4755333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvapt:	Enthalpy of vaporization at a given temperature
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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