

trans-1-Methyl-1,2-dicyclopropylcyclopropane

Inchi:	InChI=1S/C10H16/c1-10(8-4-5-8)6-9(10)7-2-3-7/h7-9H,2-6H2,1H3/t9-,10-/m1/s1
InchiKey:	GTKAAVZEFUFXDD-NXEZZACHSA-N
Formula:	C10H16
SMILES:	CC1(C2CC2)CC1C1CC1
Mol. weight [g/mol]:	136.23
CAS:	150895-64-0

Physical Properties

Property code	Value	Unit	Source
chl	-6353.70 ± 1.10	kJ/mol	NIST Webbook
gf	202.37	kJ/mol	Joback Method
hf	179.20 ± 1.20	kJ/mol	NIST Webbook
hfl	131.90 ± 1.20	kJ/mol	NIST Webbook
hfus	10.83	kJ/mol	Joback Method
hvap	47.30	kJ/mol	NIST Webbook
log10ws	-2.73		Crippen Method
logp	2.833		Crippen Method
mcvol	119.180	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
tb	443.99	K	Joback Method
tc	658.52	K	Joback Method
tf	275.94	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.62	J/mol×K	443.99	Joback Method
cpg	294.10	J/mol×K	479.74	Joback Method
cpg	312.83	J/mol×K	515.50	Joback Method
cpg	330.00	J/mol×K	551.25	Joback Method
cpg	345.77	J/mol×K	587.01	Joback Method
cpg	360.35	J/mol×K	622.76	Joback Method
cpg	373.92	J/mol×K	658.52	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=C150895640&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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