

Tetracyclo[5.2.1.0^{2,6}.0^{3,5}

Other names:	Tetracyclo[5.2.1.0
Inchi:	InChI=1S/C10H14/c1-2-6-3-5(1)9-7-4-8(7)10(6)9/h5-10H,1-4H2
InchiKey:	RQMXABDSHYTRIF-UHFFFAOYSA-N
Formula:	C10H14
SMILES:	C1CC2CC1C1C3CC3C21
Mol. weight [g/mol]:	134.22
CAS:	53862-36-5

Physical Properties

Property code	Value	Unit	Source
gf	285.10	kJ/mol	Joback Method
hf	13.11	kJ/mol	Joback Method
hfus	20.54	kJ/mol	Joback Method
hvap	36.54	kJ/mol	Joback Method
ie	9.20 ± 0.03	eV	NIST Webbook
log10ws	-2.14		Crippen Method
logp	2.298		Crippen Method
mcvol	108.320	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	437.28	K	Joback Method
tc	642.66	K	Joback Method
tf	272.78	K	Joback Method
vc	0.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.25	J/mol×K	437.28	Joback Method
cpg	344.49	J/mol×K	608.43	Joback Method
cpg	330.07	J/mol×K	574.20	Joback Method
cpg	314.45	J/mol×K	539.97	Joback Method
cpg	297.53	J/mol×K	505.74	Joback Method
cpg	279.17	J/mol×K	471.51	Joback Method
cpg	357.85	J/mol×K	642.66	Joback Method

dvisc	0.0025990	Paxs	437.28	Joback Method
dvisc	0.0019936	Paxs	409.86	Joback Method
dvisc	0.0014722	Paxs	382.45	Joback Method
dvisc	0.0010374	Paxs	355.03	Joback Method
dvisc	0.0006894	Paxs	327.61	Joback Method
dvisc	0.0004252	Paxs	300.20	Joback Method
dvisc	0.0002380	Paxs	272.78	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=C53862365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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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