

Tetracyclo[3.2.0.0^{2,7}.0^{4,6}

Other names:	Tetracyclo[3.2.0.0
Inchi:	InChI=1S/C15H12/c1(2-4-8-9(4)11-5(2)10(8)11)3-6-12-13(6)15-7(3)14(12)15/h4-15H
InchiKey:	XFFRMGONLYTZSN-UHFFFAOYSA-N
Formula:	C15H12
SMILES:	C(=C1C2C3C2C2C1C32)=C1C2C3C2C2C1C32
Mol. weight [g/mol]:	192.26
CAS:	73050-57-4

Physical Properties

Property code	Value	Unit	Source
gf	790.56	kJ/mol	Joback Method
hf	407.33	kJ/mol	Joback Method
hfus	47.54	kJ/mol	Joback Method
hvap	47.38	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
log10ws	-2.09		Crippen Method
logp	1.941		Crippen Method
mcvol	126.730	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	547.53	K	Joback Method
tc	756.42	K	Joback Method
tf	452.88	K	Joback Method
vc	0.574	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.52	J/molxK	547.53	Joback Method
cpg	426.19	J/molxK	582.35	Joback Method
cpg	441.21	J/molxK	617.16	Joback Method
cpg	454.86	J/molxK	651.98	Joback Method
cpg	467.39	J/molxK	686.79	Joback Method
cpg	479.07	J/molxK	721.61	Joback Method
cpg	490.17	J/molxK	756.42	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=C73050574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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