Tetracyclo[3.2.0.02,7.04,6]heptane,3,3'-methanete

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

Physical Properties

Property code	Value	Unit	Source
hfus	47.54	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
logp	1.941		Crippen Method
mcvol	126.730	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.52	J/mol×K	547.53	Joback Method
cpg	426.19	J/mol×K	582.35	Joback Method
cpg	441.21	J/mol×K	617.16	Joback Method
cpg	454.86	J/mol×K	651.98	Joback Method
cpg	467.39	J/mol×K	686.79	Joback Method
cpg	479.07	J/mol×K	721.61	Joback Method
cpg	490.17	J/mol×K	756.42	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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?ID=C73050574&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume