Tetracyclo[6.1.0.0^{2,4}.0^{5,7}

Other names: Tetracyclo[6.1.0.0
Inchi: InChI=1S/C9H12/c1-4-5(1)7-3-9(7)8-2-6(4)8/h4-9H,1-3H2
InchiKey: KSRIBXUCAQAWHL-UHFFFAOYSA-N
Formula: C9H12
SMILES: C1C2C3CC3C3CC3C12
Mol. weight [g/mol]: 120.19
CAS: 37831-90-6

Physical Properties

Property code	Value	Unit	Source
gf	288.78	kJ/mol	Joback Method
hf	39.91	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	34.15	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	1.908		Crippen Method
mcvol	94.230	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	410.13	K	Joback Method
tc	609.46	K	Joback Method
tf	265.03	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.86	J/mol×K	410.13	Joback Method
cpg	293.88	J/mol×K	576.24	Joback Method
cpg	280.79	J/mol×K	543.02	Joback Method
cpg	266.56	J/mol×K	509.80	Joback Method
cpg	251.07	J/mol×K	476.57	Joback Method
cpg	234.21	J/mol×K	443.35	Joback Method
cpg	305.94	J/mol×K	609.46	Joback Method

dvisc	0.0018785	Pa×s	410.13	Joback Method
dvisc	0.0013753	Pa×s	385.95	Joback Method
dvisc	0.0009657	Pa×s	361.76	Joback Method
dvisc	0.0006447	Pa×s	337.58	Joback Method
dvisc	0.0004043	Pa×s	313.40	Joback Method
dvisc	0.0002345	Pa×s	289.21	Joback Method
dvisc	0.0001232	Pa×s	265.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37831906&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

Latest version available from:
https://www.chemeo.com/cid/33-692-7/Tetracyclo-6-1-0-0-sup-2-4-sup-0-sup-5-7-sup-nonane-1and-945-2and-945-4a
Generated by Cheméo on 2024-04-29 12:02:05.694009369 +0000 UTC m=+16681374.614586684.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.