Tricyclo[4.2.0.0^{2,5}]octane,1,2,5,6-tetr

Other names: Tricyclo[4.2.0.0
Inchi: InChI=1S/C16H20/c1-9-10(2)14(6)13(9,5)15(7)11(3)12(4)16(14,15)8/h1-4H2,5-8H3
InchiKey: RRNQSOQWCKWZLJ-UHFFFAOYSA-N
Formula: C16H20
SMILES: C=C1C(=C)C2(C)C1(C)C1(C)C(=C)C(=C)C21C
Mol. weight [g/mol]: 212.33
CAS: 34101-24-1

Physical Properties

Property code	Value	Unit	Source
gf	460.84	kJ/mol	Joback Method
hf	228.57	kJ/mol	Joback Method
hfus	4.94	kJ/mol	Joback Method
hvap	46.50	kJ/mol	Joback Method
ie	8.10 ± 0.02	eV	NIST Webbook
log10ws	-4.65		Crippen Method
logp	4.277		Crippen Method
mcvol	186.520	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	574.36	K	Joback Method
tc	794.83	K	Joback Method
tf	473.50	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.52	J/mol×K	574.36	Joback Method
cpg	499.42	J/mol×K	611.11	Joback Method
cpg	514.21	J/mol×K	647.85	Joback Method
cpg	528.36	J/mol×K	684.60	Joback Method
cpg	542.33	J/mol×K	721.34	Joback Method
cpg	556.59	J/mol×K	758.09	Joback Method
cpg	571.59	J/mol×K	794.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34101241&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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