Tricyclo[4.2.0.02,5]octane, syn-

Inchi: InChI=1S/C8H12/c1-2-6-5(1)7-3-4-8(6)7/h5-8H,1-4H2/t5-,6+,7-,8+
InchiKey: YTZCZYFFHKYOBJ-KVFPUHGPSA-N
Formula: C8H12
SMILES: C1CC2C1C1CCC21
Mol. weight [g/mol]: 108.18
CAS: 28636-10-4

Physical Properties

Property code	Value	Unit	Source
chl	-5056.00 ± 4.00	kJ/mol	NIST Webbook
gf	203.12	kJ/mol	Joback Method
hf	235.00 ± 4.20	kJ/mol	NIST Webbook
hfl	193.00 ± 4.00	kJ/mol	NIST Webbook
hfus	14.05	kJ/mol	Joback Method
hvap	41.80 ± 1.70	kJ/mol	NIST Webbook
hvap	42.00 ± 2.00	kJ/mol	NIST Webbook
hvap	42.00	kJ/mol	NIST Webbook
ie	9.18	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.052		Crippen Method
mcvol	91.000	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	393.72	K	Joback Method
tc	594.92	K	Joback Method
tf	233.02	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.89	J/mol×K	393.72	Joback Method
cpg	204.36	J/mol×K	427.25	Joback Method
cpg	220.54	J/mol×K	460.79	Joback Method
cpg	235.52	J/mol×K	494.32	Joback Method

cpg	249.40	J/mol×K	527.85	Joback Method
cpg	262.25	J/mol×K	561.38	Joback Method
cpg	274.16	J/mol×K	594.92	Joback Method
dvisc	0.0001567	Pa×s	233.02	Joback Method
dvisc	0.0002381	Pa×s	259.80	Joback Method
dvisc	0.0003344	Pa×s	286.59	Joback Method
dvisc	0.0004433	Pa×s	313.37	Joback Method
dvisc	0.0005621	Pa×s	340.15	Joback Method
dvisc	0.0006884	Pa×s	366.94	Joback Method
dvisc	0.0008202	Pa×s	393.72	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28636104&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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