

Tricyclo[2.2.1.0(2,6)]heptane

Other names:	Nortricyclane Nortricyclen Nortricyclene Tricyclo[2.2.1.0dimethyl2dimethyl,dimethyl6]heptane Tricyclo[2.2.1.0^2^,^6]heptane Tricyclo[2.2.1.0(2.6)]heptane
Inchi:	InChI=1S/C7H10/c1-4-2-6-5(1)7(6)3-4/h4-7H,1-3H2
InchiKey:	BYBGSCXPMGPLFP-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	C1C2CC3C1C3C2
Mol. weight [g/mol]:	94.15
CAS:	279-19-6

Physical Properties

Property code	Value	Unit	Source
chl	-4207.80 ± 2.20	kJ/mol	NIST Webbook
chl	-4227.10 ± 2.00	kJ/mol	NIST Webbook
chs	-4214.80 ± 1.00	kJ/mol	NIST Webbook
gf	206.80	kJ/mol	Joback Method
hf	70.20 ± 1.60	kJ/mol	NIST Webbook
hf	62.00 ± 2.30	kJ/mol	NIST Webbook
hf	99.60	kJ/mol	NIST Webbook
hf	84.50	kJ/mol	NIST Webbook
hf	82.10 ± 2.10	kJ/mol	NIST Webbook
hf	78.20	kJ/mol	NIST Webbook
hfl	43.40 ± 2.00	kJ/mol	NIST Webbook
hfl	24.00 ± 2.20	kJ/mol	NIST Webbook
hfs	31.00 ± 1.10	kJ/mol	NIST Webbook
hfus	13.56	kJ/mol	Joback Method
hsub	38.70 ± 0.70	kJ/mol	NIST Webbook
hsub	39.20 ± 1.10	kJ/mol	NIST Webbook
hsub	39.20	kJ/mol	NIST Webbook
hsub	39.20 ± 1.10	kJ/mol	NIST Webbook
hvap	38.00	kJ/mol	NIST Webbook
hvap	38.00 ± 0.08	kJ/mol	NIST Webbook
hvap	38.70 ± 0.70	kJ/mol	NIST Webbook
hvap	38.50	kJ/mol	NIST Webbook

hvap	38.70	kJ/mol	NIST Webbook
ie	9.37	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	8.92 ± 0.01	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.662		Crippen Method
mcvol	76.910	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	857.00		NIST Webbook
rinpol	857.00		NIST Webbook
tb	366.57	K	Joback Method
tc	560.65	K	Joback Method
tf	225.27	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.81	J/mol×K	560.65	Joback Method
cpg	148.43	J/mol×K	366.57	Joback Method
cpg	215.38	J/mol×K	528.30	Joback Method
cpg	204.06	J/mol×K	495.96	Joback Method
cpg	191.80	J/mol×K	463.61	Joback Method
cpg	178.49	J/mol×K	431.26	Joback Method
cpg	164.06	J/mol×K	398.92	Joback Method
cps	110.20	J/mol×K	297.00	NIST Webbook
cps	129.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0000673	Pa×s	225.27	Joback Method
dvisc	0.0004537	Pa×s	343.02	Joback Method
dvisc	0.0003466	Pa×s	319.47	Joback Method
dvisc	0.0002537	Pa×s	295.92	Joback Method
dvisc	0.0001760	Pa×s	272.37	Joback Method
dvisc	0.0001139	Pa×s	248.82	Joback Method
dvisc	0.0005736	Pa×s	366.57	Joback Method
hvapt	38.30	kJ/mol	319.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C279196&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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