Tetracyclo[3.2.0.0(2,7).0(4,6)]heptane

Other names:	Quadricyclane
	Tetracyclo[2.2.1.0(2,6).0(3,5)]heptane
	[2.2.1.02,6.03,5]Quadricycloheptane
	tetracyclo[2.2.1.02,6.03,5]heptane
Inchi:	InChI=1S/C7H8/c1-2-4-5(2)7-3(1)6(4)7/h2-7H,1H2
InchiKey:	DGZUEIPKRRSMGK-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C1C2C3C2C2C1C32
Mol. weight [g/mol]:	92.14
CAS:	278-06-8

Physical Properties

Property code	Value	Unit	Source
chl	-4114.30 ± 1.10	kJ/mol	NIST Webbook
chl	-4200.00 ± 2.20	kJ/mol	NIST Webbook
gf	296.14	kJ/mol	Joback Method
hf	333.00	kJ/mol	NIST Webbook
hf	339.10 ± 2.30	kJ/mol	NIST Webbook
hf	325.00 ± 4.20	kJ/mol	NIST Webbook
hf	253.30 ± 1.10	kJ/mol	NIST Webbook
hf	336.00	kJ/mol	NIST Webbook
hfl	302.10 ± 2.20	kJ/mol	NIST Webbook
hfl	216.30 ± 1.10	kJ/mol	NIST Webbook
hfus	19.07	kJ/mol	Joback Method
hvap	37.00 ± 0.80	kJ/mol	NIST Webbook
hvap	37.00 ± 0.20	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
hvap	37.90 ± 0.10	kJ/mol	NIST Webbook
hvap	37.90 ± 0.10	kJ/mol	NIST Webbook
hvap	37.00	kJ/mol	NIST Webbook
hvap	37.00 ± 0.80	kJ/mol	NIST Webbook
hvap	37.85 ± 0.44	kJ/mol	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	8.33	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-0.88		Crippen Method
logp	1.128		Crippen Method

mcvol	66.050	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	355.83	K	Joback Method
tc	541.30	K	Joback Method
tf	249.53	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.29	J/mol×K	417.65	Joback Method
cpg	137.29	J/mol×K	355.83	Joback Method
cpg	178.87	J/mol×K	448.56	Joback Method
cpg	190.29	J/mol×K	479.47	Joback Method
cpg	200.66	J/mol×K	510.39	Joback Method
cpg	210.09	J/mol×K	541.30	Joback Method
cpg	152.46	J/mol×K	386.74	Joback Method
cpl	157.60	J/mol×K	298.15	NIST Webbook
cpl	139.10	J/mol×K	297.00	NIST Webbook
dvisc	0.0005902	Pa×s	355.83	Joback Method
dvisc	0.0002585	Pa×s	320.40	Joback Method
dvisc	0.0001591	Pa×s	302.68	Joback Method
dvisc	0.0000922	Pa×s	284.96	Joback Method
dvisc	0.0000497	Pa×s	267.25	Joback Method
dvisc	0.0003992	Pa×s	338.11	Joback Method
dvisc	0.0000245	Pa×s	249.53	Joback Method
hfust	1.09	kJ/mol	228.00	NIST Webbook
hfust	7.20	kJ/mol	180.00	NIST Webbook
hfust	1.09	kJ/mol	228.00	NIST Webbook
hvapt	37.30 ± 0.80	kJ/mol	337.00	NIST Webbook
sfust	4.80	J/mol×K	228.00	NIST Webbook
sfust	40.00	J/mol×K	180.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47079e+01
Coeff. B	-3.38474e+03
Coeff. C	-4.42240e+01
Temperature range (K), min.	278.94
Temperature range (K), max.	404.44

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C278068&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid 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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume