Cubane

Inchi: InChI=1S/C8H8/c1-2-5-3(1)7-4(1)6(2)8(5)7/h1-8H
InchiKey: TXWRERCHRDBNLG-UHFFFAOYSA-N
Formula: C8H8
SMILES: C12C3C4C1C1C2C3C41
Mol. weight [g/mol]: 104.15
CAS: 277-10-1

Physical Properties

Property code	Value	Unit	Source
affp	859.90	kJ/mol	NIST Webbook
basg	833.60	kJ/mol	NIST Webbook
chs	-4833.27	kJ/mol	NIST Webbook
gf	381.80	kJ/mol	Joback Method
hf	622.20 ± 4.20	kJ/mol	NIST Webbook
hfs	542.00 ± 3.00	kJ/mol	NIST Webbook
hfus	25.06	kJ/mol	Joback Method
hsub	80.30 ± 1.60	kJ/mol	NIST Webbook
hsub	80.20	kJ/mol	NIST Webbook
hsub	55.20 ± 2.00	kJ/mol	NIST Webbook
hvap	44.60 ± 0.80	kJ/mol	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
ie	8.40 ± 0.10	eV	NIST Webbook
ie	8.64 ± 0.10	eV	NIST Webbook
ie	8.74	eV	NIST Webbook
ie	8.74 ± 0.15	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-0.71		Crippen Method
logp	0.984		Crippen Method
mcvol	69.280	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	372.24	K	Joback Method
tc	556.70	K	Joback Method
tf	281.54	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.50	J/mol×K	372.24	Joback Method
cpg	230.51	J/mol×K	525.95	Joback Method
cpg	219.71	J/mol×K	495.21	Joback Method
cpg	207.73	J/mol×K	464.47	Joback Method
cpg	194.45	J/mol×K	433.73	Joback Method
cpg	179.75	J/mol×K	402.98	Joback Method
cpg	240.26	J/mol×K	556.70	Joback Method
dvisc	0.0001014	Pa×s	296.66	Joback Method
dvisc	0.0001873	Pa×s	311.77	Joback Method
dvisc	0.0003267	Pa×s	326.89	Joback Method
dvisc	0.0005426	Pa×s	342.01	Joback Method
dvisc	0.0008633	Pa×s	357.12	Joback Method
dvisc	0.0000514	Pa×s	281.54	Joback Method
dvisc	0.0013227	Pa×s	372.24	Joback Method
hfust	8.70	kJ/mol	404.90	NIST Webbook
hfust	5.94	kJ/mol	394.00	NIST Webbook
hfust	8.70	kJ/mol	404.90	NIST Webbook
hsubt	80.00 ± 2.00	kJ/mol	239.00	NIST Webbook
sfust	21.49	J/mol×K	404.90	NIST Webbook
sfust	15.08	J/mol×K	394.00	NIST Webbook

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=C277101&Units=SI

Legend

affp: Proton affinity

basg:	Gas basicity
chs:	Standard solid 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
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/24-410-9/Cubane.pdf

Generated by Cheméo on 2024-10-12 09:03:26.105288216 +0000 UTC m=+3304668.742257465.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.