CD2

Inchi: InChI=1S/CH2/h1H2/i1D2
InchiKey: HZVOZRGWRWCICA-DICFDUPASA-N
Formula: CD2
SMILES: [CH2]
Mol. weight [g/mol]: 16.04
CAS: 14863-68-4

Physical Properties

Property code	Value	Unit	Source
ea	1.04 ± 0.01	eV	NIST Webbook
ea	0.65 ± 0.01	eV	NIST Webbook
gf	62.30	kJ/mol	Joback Method
hf	47.65	kJ/mol	Joback Method
hfus	1.71	kJ/mol	Joback Method
hvap	17.53	kJ/mol	Joback Method
log10ws	0.20		Crippen Method
logp	0.327		Crippen Method
mcvol	20.650	ml/mol	McGowan Method
pc	6653.02	kPa	Joback Method
tb	220.88	K	Joback Method
tc	366.98	K	Joback Method
tf	133.77	K	Joback Method
vc	0.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	9.15	J/mol×K	220.88	Joback Method
cpg	12.38	J/mol×K	245.23	Joback Method
cpg	15.28	J/mol×K	269.58	Joback Method
cpg	17.86	J/mol×K	293.93	Joback Method
cpg	20.14	J/mol×K	318.28	Joback Method
cpg	22.14	J/mol×K	342.63	Joback Method
cpg	23.88	J/mol×K	366.98	Joback Method

dvisc	0.0000036	Pa×s	133.77	Joback Method
dvisc	0.0000053	Pa×s	148.29	Joback Method
dvisc	0.0000071	Pa×s	162.81	Joback Method
dvisc	0.0000092	Pa×s	177.32	Joback Method
dvisc	0.0000114	Pa×s	191.84	Joback Method
dvisc	0.0000137	Pa×s	206.36	Joback Method
dvisc	0.0000160	Pa×s	220.88	Joback Method

Sources

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=C14863684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
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