

Cyclopropyl radical

Inchi: InChI=1S/C3H5/c1-2-3-1/h1H,2-3H2
InchiKey: XIPUIGNIDKXJU-UHFFFAOYSA-N
Formula: C3H5
SMILES: [CH]1CC1
Mol. weight [g/mol]: 41.07
CAS: 2417-82-5

Physical Properties

Property code	Value	Unit	Source
affp	738.90	kJ/mol	NIST Webbook
basg	702.00	kJ/mol	NIST Webbook
ea	0.36 ± 0.09	eV	NIST Webbook
ea	0.51 ± 0.21	eV	NIST Webbook
ea	0.40 ± 0.07	eV	NIST Webbook
gf	87.51	kJ/mol	Joback Method
hf	23.36	kJ/mol	Joback Method
hfpi	1070.00	kJ/mol	NIST Webbook
hfus	3.34	kJ/mol	Joback Method
hvap	22.04	kJ/mol	Joback Method
ie	8.18 ± 0.03	eV	NIST Webbook
ie	8.68 ± 0.02	eV	NIST Webbook
log10ws	-0.58		Crippen Method
logp	0.984		Crippen Method
mcvol	40.120	ml/mol	McGowan Method
pc	5636.27	kPa	Joback Method
tb	274.08	K	Joback Method
tc	446.36	K	Joback Method
tf	157.88	K	Joback Method
vc	0.151	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	40.47	J/mol×K	274.08	Joback Method

cpg	74.24	J/mol×K	417.65	Joback Method
cpg	68.53	J/mol×K	388.93	Joback Method
cpg	62.33	J/mol×K	360.22	Joback Method
cpg	55.61	J/mol×K	331.51	Joback Method
cpg	48.33	J/mol×K	302.79	Joback Method
cpg	79.49	J/mol×K	446.36	Joback Method
dvisc	0.0001003	Paxs	274.08	Joback Method
dvisc	0.0000903	Paxs	254.71	Joback Method
dvisc	0.0000800	Paxs	235.35	Joback Method
dvisc	0.0000693	Paxs	215.98	Joback Method
dvisc	0.0000583	Paxs	196.61	Joback Method
dvisc	0.0000473	Paxs	177.25	Joback Method
dvisc	0.0000364	Paxs	157.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2417825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfpi:	Enthalpy of formation of positive ion 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

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