

Propargyl radical

Inchi:	InChI=1S/C3H3/c1-3-2/h1H,2H2
InchiKey:	DITHIFQMPPCBCU-UHFFFAOYSA-N
Formula:	C3H3
SMILES:	C#C[CH2]
Mol. weight [g/mol]:	39.06
CAS:	2932-78-7

Physical Properties

Property code	Value	Unit	Source
affp	741.00	kJ/mol	NIST Webbook
basg	708.50	kJ/mol	NIST Webbook
gf	249.83	kJ/mol	Joback Method
hf	339.00 ± 4.00	kJ/mol	NIST Webbook
hfpi	1180.00	kJ/mol	NIST Webbook
hfus	8.18	kJ/mol	Joback Method
hvap	21.98	kJ/mol	Joback Method
ie	8.68	eV	NIST Webbook
ie	8.67 ± 0.02	eV	NIST Webbook
log10ws	-0.48		Crippen Method
logp	0.454		Crippen Method
mvol	42.380	ml/mol	McGowan Method
pc	5791.74	kPa	Joback Method
tb	257.46	K	Joback Method
tc	424.70	K	Joback Method
tf	186.91	K	Joback Method
vc	0.157	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	50.12	J/mol×K	257.46	Joback Method
cpg	54.18	J/mol×K	285.33	Joback Method
cpg	57.90	J/mol×K	313.21	Joback Method
cpg	61.31	J/mol×K	341.08	Joback Method

cpg	64.43	J/mol×K	368.95	Joback Method
cpg	67.28	J/mol×K	396.83	Joback Method
cpg	69.88	J/mol×K	424.70	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=C2932787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
mccvol:	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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