1-Butyn-3-yl radical

Inchi: InChI=1S/C4H5/c1-3-4-2/h1,4H,2H3
InchiKey: ULVFVBQUCTUAPR-UHFFFAOYSA-N
Formula: C4H5
SMILES: C#C[CH]C
Mol. weight [g/mol]: 53.08
CAS: 3315-42-2

Physical Properties

Property code	Value	Unit	Source
gf	255.81	kJ/mol	Joback Method
hf	216.54	kJ/mol	Joback Method
hfpi	1080.00	kJ/mol	NIST Webbook
hfus	7.25	kJ/mol	Joback Method
hvap	23.82	kJ/mol	Joback Method
ie	7.97	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	0.844		Crippen Method
mcvol	56.470	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
tb	279.90	K	Joback Method
tc	453.85	K	Joback Method
tf	183.18	K	Joback Method
vc	0.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.81	J/mol×K	279.90	Joback Method
cpg	80.77	J/mol×K	308.89	Joback Method
cpg	86.31	J/mol×K	337.88	Joback Method
cpg	91.45	J/mol×K	366.87	Joback Method
cpg	96.23	J/mol×K	395.86	Joback Method
cpg	100.65	J/mol×K	424.86	Joback Method
cpg	104.76	J/mol×K	453.85	Joback Method

Sources

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=C3315422&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume