

But-2-yn-1-yl radical

Inchi:	InChI=1S/C4H5/c1-3-4-2/h1H2,2H3
InchiKey:	LSOBPYSQSPIQJF-UHFFFAOYSA-N
Formula:	C4H5
SMILES:	[CH2]C#CC
Mol. weight [g/mol]:	53.08
CAS:	82252-88-8

Physical Properties

Property code	Value	Unit	Source
gf	237.98	kJ/mol	Joback Method
hf	202.22	kJ/mol	Joback Method
hfpi	1050.00	kJ/mol	NIST Webbook
hfus	10.92	kJ/mol	Joback Method
hvap	26.50	kJ/mol	Joback Method
ie	7.95	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	0.844		Crippen Method
mcvol	56.470	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
tb	299.22	K	Joback Method
tc	483.91	K	Joback Method
tf	257.31	K	Joback Method
vc	0.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	72.92	J/molxK	299.22	Joback Method
cpg	78.45	J/molxK	330.00	Joback Method
cpg	83.62	J/molxK	360.78	Joback Method
cpg	88.46	J/molxK	391.57	Joback Method
cpg	92.99	J/molxK	422.35	Joback Method
cpg	97.24	J/molxK	453.13	Joback Method
cpg	101.21	J/molxK	483.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82252888&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

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

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