Allyl radical

Inchi: InChI=1S/C3H5/c1-3-2/h3H,1-2H2
InchiKey: RMRFFCXPLWYOOY-UHFFFAOYSA-N
Formula: C3H5
SMILES: [CH2]C=C
Mol. weight [g/mol]: 41.07
CAS: 1981-80-2

Physical Properties

Property code	Value	Unit	Source
affp	736.00	kJ/mol	NIST Webbook
basg	707.40	kJ/mol	NIST Webbook
ea	0.55 ± 0.05	eV	NIST Webbook
ea	0.36 ± 0.02	eV	NIST Webbook
ea	0.47 ± 0.10	eV	NIST Webbook
ea	0.48 ± 0.01	eV	NIST Webbook
gf	114.60	kJ/mol	Joback Method
hf	171.00 ± 3.00	kJ/mol	NIST Webbook
hfpi	945.60	kJ/mol	NIST Webbook
hfpiz	957.70	kJ/mol	NIST Webbook
hfus	3.93	kJ/mol	Joback Method
hvap	21.46	kJ/mol	Joback Method
ie	8.10 ± 0.10	eV	NIST Webbook
ie	8.07 ± 0.03	eV	NIST Webbook
ie	8.13 ± 0.02	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.18 ± 0.07	eV	NIST Webbook
log10ws	-0.54		Crippen Method
logp	1.006		Crippen Method
mcvol	46.680	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
tb	264.02	K	Joback Method
tc	423.29	K	Joback Method
tf	138.18	K	Joback Method
vc	0.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	51.95	J/mol×K	264.02	Joback Method
cpg	57.30	J/mol×K	290.56	Joback Method
cpg	62.32	J/mol×K	317.11	Joback Method
cpg	67.01	J/mol×K	343.65	Joback Method
cpg	71.41	J/mol×K	370.20	Joback Method
cpg	75.52	J/mol×K	396.74	Joback Method
cpg	79.36	J/mol×K	423.29	Joback Method
dvisc	0.0001319	Pa×s	138.18	Joback Method
dvisc	0.0001229	Pa×s	159.15	Joback Method
dvisc	0.0001165	Pa×s	180.13	Joback Method
dvisc	0.0001116	Pa×s	201.10	Joback Method
dvisc	0.0001078	Pa×s	222.07	Joback Method
dvisc	0.0001048	Pa×s	243.05	Joback Method
dvisc	0.0001023	Pa×s	264.02	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=C1981802&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

hfpiz:	Enthalpy of formation of positive ion at 0K
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