2-Methylallyl radical

Inchi: InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3
InchiKey: LJXPWUAAAAXJBX-UHFFFAOYSA-N
Formula: C4H7
SMILES: [CH2]C(=C)C
Mol. weight [g/mol]: 55.10
CAS: 15157-95-6

Physical Properties

Property code	Value	Unit	Source
affp	778.00	kJ/mol	NIST Webbook
basg	747.30	kJ/mol	NIST Webbook
ea	0.51 ± 0.01	eV	NIST Webbook
ea	0.36 ± 0.13	eV	NIST Webbook
gf	114.47	kJ/mol	Joback Method
hf	45.56	kJ/mol	Joback Method
hfus	5.21	kJ/mol	Joback Method
hvap	23.76	kJ/mol	Joback Method
ie	7.89	eV	NIST Webbook
ie	7.88 ± 0.05	eV	NIST Webbook
ie	7.95 ± 0.02	eV	NIST Webbook
ie	7.90 ± 0.02	eV	NIST Webbook
log10ws	-0.96		Crippen Method
logp	1.397		Crippen Method
mcvol	60.770	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	286.78	K	Joback Method
tc	451.69	K	Joback Method
tf	135.49	K	Joback Method
vc	0.233	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.84	J/mol×K	286.78	Joback Method

cpg	85.85	J/mol×K	314.27	Joback Method
cpg	92.45	J/mol×K	341.75	Joback Method
cpg	98.66	J/mol×K	369.24	Joback Method
cpg	104.50	J/mol×K	396.72	Joback Method
cpg	109.99	J/mol×K	424.21	Joback Method
cpg	115.16	J/mol×K	451.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15157956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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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