But-3-en-1-yl radical

Inchi: InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2
InchiKey: UHURJXXAXXMMLW-UHFFFAOYSA-N
Formula: C4H7
SMILES: [CH2]CC=C
Mol. weight [g/mol]: 55.10
CAS: 2154-62-3

Physical Properties

Property code	Value	Unit	Source
ea	0.09 ± 0.12	eV	NIST Webbook
gf	123.02	kJ/mol	Joback Method
hf	55.35	kJ/mol	Joback Method
hfus	6.52	kJ/mol	Joback Method
hvap	23.68	kJ/mol	Joback Method
ie	8.04 ± 0.03	eV	NIST Webbook
ie	8.47 ± 0.05	eV	NIST Webbook
log10ws	-0.96		Crippen Method
logp	1.397		Crippen Method
mcvol	60.770	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	286.90	K	Joback Method
tc	448.29	K	Joback Method
tf	149.45	K	Joback Method
vc	0.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.73	J/mol×K	286.90	Joback Method
cpg	109.44	J/mol×K	421.39	Joback Method
cpg	104.01	J/mol×K	394.49	Joback Method
cpg	98.24	J/mol×K	367.60	Joback Method
cpg	92.12	J/mol×K	340.70	Joback Method
cpg	85.62	J/mol×K	313.80	Joback Method

cpg	114.56	J/mol×K	448.29	Joback Method
dvisc	0.0001527	Pa×s	286.90	Joback Method
dvisc	0.0001607	Pa×s	263.99	Joback Method
dvisc	0.0001707	Pa×s	241.08	Joback Method
dvisc	0.0001836	Pa×s	218.17	Joback Method
dvisc	0.0002009	Pa×s	195.27	Joback Method
dvisc	0.0002252	Pa×s	172.36	Joback Method
dvisc	0.0002615	Pa×s	149.45	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=C2154623&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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