1-Buten-3-yl radical

Other names: 1-Buten-3-yl radical
Inchi: InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3
InchiKey: CRPTXKKKIGGDBX-UHFFFAOYSA-N
Formula: C4H7
SMILES: C=C[CH]C
Mol. weight [g/mol]: 55.10

Physical Properties

Property code	Value	Unit	Source
af	0.1904		Cheméo Relay (1.0)
gf	120.58	kJ/mol	Joback Method
hf	64.84	kJ/mol	Cheméo Relay (1.0)
hfus	3.00	kJ/mol	Joback Method
hvap	21.11	kJ/mol	Cheméo Relay (1.0)
ie	7.54	eV	NIST Webbook
ie	7.67 ± 0.02	eV	NIST Webbook
ie	7.49 ± 0.02	eV	NIST Webbook
log10ws	-1.42		Cheméo Relay (1.0)
logp	1.397		Crippen Method
mcvol	60.770	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
tb	272.53	K	Cheméo Relay (1.0)
tc	404.43	K	Cheméo Relay (1.0)
tf	110.61	K	Cheméo Relay (1.0)
vc	0.230	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.36	J/mol×K	286.46	Joback Method
cpg	85.53	J/mol×K	314.05	Joback Method
cpg	92.28	J/mol×K	341.63	Joback Method
cpg	98.64	J/mol×K	369.22	Joback Method
cpg	104.62	J/mol×K	396.80	Joback Method

cpg	110.25	J/mol×K	424.39	Joback Method
cpg	115.53	J/mol×K	451.98	Joback Method
dvisc	0.0003434	Pa×s	134.45	Joback Method
dvisc	0.0002695	Pa×s	159.78	Joback Method
dvisc	0.0002260	Pa×s	185.12	Joback Method
dvisc	0.0001977	Pa×s	210.46	Joback Method
dvisc	0.0001780	Pa×s	235.79	Joback Method
dvisc	0.0001635	Pa×s	261.12	Joback Method
dvisc	0.0001525	Pa×s	286.46	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65338310&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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