1-Butyl radical

Inchi: InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3
InchiKey: WPWHSFAFEBZWBB-UHFFFAOYSA-N
Formula: C4H9
SMILES: [CH2]CCC
Mol. weight [g/mol]: 57.11
CAS: 2492-36-6

Physical Properties

Property code	Value	Unit	Source
gf	35.18	kJ/mol	Joback Method
hf	-70.08	kJ/mol	Joback Method
hfus	7.80	kJ/mol	Joback Method
hvap	24.35	kJ/mol	Joback Method
ie	8.01 ± 0.05	eV	NIST Webbook
ie	8.01 ± 0.05	eV	NIST Webbook
ie	8.50 ± 0.04	eV	NIST Webbook
ie	8.02 ± 0.04	eV	NIST Webbook
log10ws	-1.11		Crippen Method
logp	1.621		Crippen Method
mcvol	65.070	ml/mol	McGowan Method
pc	4119.70	kPa	Joback Method
tb	290.22	K	Joback Method
tc	448.35	K	Joback Method
tf	151.21	K	Joback Method
vc	0.251	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.91	J/mol×K	290.22	Joback Method
cpg	123.77	J/mol×K	421.99	Joback Method
cpg	117.67	J/mol×K	395.64	Joback Method
cpg	111.25	J/mol×K	369.28	Joback Method
cpg	104.49	J/mol×K	342.93	Joback Method

cpg	97.38	J/mol×K	316.57	Joback Method
cpg	129.57	J/mol×K	448.35	Joback Method
dvisc	0.0001716	Pa×s	290.22	Joback Method
dvisc	0.0001840	Pa×s	267.05	Joback Method
dvisc	0.0001999	Pa×s	243.88	Joback Method
dvisc	0.0002210	Pa×s	220.72	Joback Method
dvisc	0.0002501	Pa×s	197.55	Joback Method
dvisc	0.0002925	Pa×s	174.38	Joback Method
dvisc	0.0003589	Pa×s	151.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2492366&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

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

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