

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	8.02 ± 0.04	eV	NIST Webbook
ie	8.01 ± 0.05	eV	NIST Webbook
ie	8.01 ± 0.05	eV	NIST Webbook
ie	8.50 ± 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/molxK	290.22	Joback Method
cpg	97.38	J/molxK	316.57	Joback Method
cpg	104.49	J/molxK	342.93	Joback Method
cpg	111.25	J/molxK	369.28	Joback Method
cpg	117.67	J/molxK	395.64	Joback Method

cpg	123.77	J/molxK	421.99	Joback Method
cpg	129.57	J/molxK	448.35	Joback Method
dvisc	0.0003589	Paxs	151.21	Joback Method
dvisc	0.0002925	Paxs	174.38	Joback Method
dvisc	0.0002501	Paxs	197.55	Joback Method
dvisc	0.0002210	Paxs	220.72	Joback Method
dvisc	0.0001999	Paxs	243.88	Joback Method
dvisc	0.0001840	Paxs	267.05	Joback Method
dvisc	0.0001716	Paxs	290.22	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=C2492366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	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

Latest version available from:

<https://www.chemeo.com/cid/25-734-9/1-Butyl-radical.pdf>

Generated by Cheméo on 2024-04-19 16:03:22.144102943 +0000 UTC m=+15831851.064680260.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.