

2-Butyl radical

Inchi: InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3
InchiKey: ULOIAOPTGWSNHU-UHFFFAOYSA-N
Formula: C4H9
SMILES: C[CH]CC
Mol. weight [g/mol]: 57.11
CAS: 2348-55-2

Physical Properties

Property code	Value	Unit	Source
ea	-0.13 ± 0.09	eV	NIST Webbook
gf	32.74	kJ/mol	Joback Method
hf	69.00 ± 2.00	kJ/mol	NIST Webbook
hfpi	766.00 ± 4.00	kJ/mol	NIST Webbook
hfus	4.27	kJ/mol	Joback Method
hvap	23.96	kJ/mol	Joback Method
ie	7.59 ± 0.03	eV	NIST Webbook
ie	7.41 ± 0.05	eV	NIST Webbook
ie	7.25 ± 0.02	eV	NIST Webbook
log10ws	-1.11		Crippen Method
logp	1.621		Crippen Method
mvol	65.070	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	289.78	K	Joback Method
tc	451.90	K	Joback Method
tf	136.21	K	Joback Method
vc	0.244	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.53	J/mol×K	289.78	Joback Method
cpg	124.64	J/mol×K	424.88	Joback Method
cpg	118.33	J/mol×K	397.86	Joback Method
cpg	111.68	J/mol×K	370.84	Joback Method

cpg	104.68	J/molxK	343.82	Joback Method
cpg	97.30	J/molxK	316.80	Joback Method
cpg	130.63	J/molxK	451.90	Joback Method
dvisc	0.0001712	Paxs	289.78	Joback Method
dvisc	0.0001875	Paxs	264.19	Joback Method
dvisc	0.0002092	Paxs	238.59	Joback Method
dvisc	0.0002398	Paxs	213.00	Joback Method
dvisc	0.0002853	Paxs	187.40	Joback Method
dvisc	0.0003585	Paxs	161.81	Joback Method
dvisc	0.0004910	Paxs	136.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2348552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfpi:	Enthalpy of formation of positive ion 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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