

i-C4H9

Inchi:	InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3/q-1
InchiKey:	RFONJRMUUALMBA-UHFFFAOYSA-N
Formula:	C4H9
SMILES:	[CH2-]C(C)C
Mol. weight [g/mol]:	57.11
CAS:	65114-21-8

Physical Properties

Property code	Value	Unit	Source
gf	32.74	kJ/mol	Joback Method
hf	-75.36	kJ/mol	Joback Method
hfus	4.27	kJ/mol	Joback Method
hvap	23.96	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.476		Crippen Method
mcvol	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	m3/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/mol×K	343.82	Joback Method
cpg	97.30	J/mol×K	316.80	Joback Method
cpg	130.63	J/mol×K	451.90	Joback Method
dvisc	0.0001712	Pa×s	289.78	Joback Method
dvisc	0.0001875	Pa×s	264.19	Joback Method

dvisc	0.0002092	Pa×s	238.59	Joback Method
dvisc	0.0002398	Pa×s	213.00	Joback Method
dvisc	0.0002853	Pa×s	187.40	Joback Method
dvisc	0.0003585	Pa×s	161.81	Joback Method
dvisc	0.0004910	Pa×s	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=C65114218&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

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
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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