

3-methylbutyl radical

Inchi:	InChI=1S/C5H11/c1-4-5(2)3/h5H,1,4H2,2-3H3
InchiKey:	TXFXGCPVIYCUIT-UHFFFAOYSA-N
Formula:	C5H11
SMILES:	[CH2]CC(C)C
Mol. weight [g/mol]:	71.14
CAS:	2492-33-3

Physical Properties

Property code	Value	Unit	Source
gf	41.16	kJ/mol	Joback Method
hf	-96.00	kJ/mol	Joback Method
hfus	6.86	kJ/mol	Joback Method
hvap	26.19	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.867		Crippen Method
mcvol	79.160	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	312.66	K	Joback Method
tc	476.09	K	Joback Method
tf	147.48	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.98	J/molxK	312.66	Joback Method
cpg	129.19	J/molxK	339.90	Joback Method
cpg	137.97	J/molxK	367.14	Joback Method
cpg	146.32	J/molxK	394.37	Joback Method
cpg	154.26	J/molxK	421.61	Joback Method
cpg	161.81	J/molxK	448.85	Joback Method
cpg	169.00	J/molxK	476.09	Joback Method
dvisc	0.0008154	Paxs	147.48	Joback Method
dvisc	0.0005525	Paxs	175.01	Joback Method

dvisc	0.0004161	Paxs	202.54	Joback Method
dvisc	0.0003354	Paxs	230.07	Joback Method
dvisc	0.0002831	Paxs	257.60	Joback Method
dvisc	0.0002469	Paxs	285.13	Joback Method
dvisc	0.0002206	Paxs	312.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2492333&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
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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