Butanal, 2-ethyl-3-methyl-

Other names:	(CH3)2CHCH(C2H5)CHO
	2-Ethylisovaleraldehyde
	2-Ethyl-3-methylbutanal
	2-Ethyl-3-methylbutyraldehyde
Inchi:	InChI=1S/C7H14O/c1-4-7(5-8)6(2)3/h5-7H,4H2,1-3H3
InchiKey:	SHGPBDQRELYPLO-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCC(C=O)C(C)C
Mol. weight [g/mol]:	114.19
CAS:	26254-92-2

Physical Properties

Property code	Value	Unit	Source
gf	-96.34	kJ/mol	Joback Method
hf	-283.95	kJ/mol	Joback Method
hfus	9.13	kJ/mol	Joback Method
hvap	37.12	kJ/mol	Joback Method
ie	9.44	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	1.868		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	407.34	K	Joback Method
tc	587.04	K	Joback Method
tf	180.65	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.96	J/mol×K	407.34	Joback Method
cpg	270.87	J/mol×K	557.09	Joback Method
cpg	260.99	J/mol×K	527.14	Joback Method
cpg	250.68	J/mol×K	497.19	Joback Method

cpg	239.91	J/mol×K	467.24	Joback Method
cpg	228.67	J/mol×K	437.29	Joback Method
cpg	280.30	J/mol×K	587.04	Joback Method
dvisc	0.0002974	Pa×s	407.34	Joback Method
dvisc	0.0004058	Pa×s	369.56	Joback Method
dvisc	0.0005942	Pa×s	331.78	Joback Method
dvisc	0.0009598	Pa×s	294.00	Joback Method
dvisc	0.0017858	Pa×s	256.21	Joback Method
dvisc	0.0041185	Pa×s	218.43	Joback Method
dvisc	0.0134730	Pa×s	180.65	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26254922&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
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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