(S)-2-methylbutanal

Inchi: InChI=1S/C5H10O/c1-3-5(2)4-6/h4-5H,3H2,1-2H3/t5-/m1/s1
InchiKey: BYGQBDHUGHBGMD-RXMQYKEDSA-N
Formula: C5H10O
SMILES: CCC(C)C=O
Mol. weight [g/mol]: 86.13
CAS: 1730-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-110.74	kJ/mol	Joback Method
hf	-237.39	kJ/mol	Joback Method
hfus	7.47	kJ/mol	Joback Method
hvap	33.06	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.231		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	402.00 ± 1.00	K	NIST Webbook
tb	364.00 ± 3.00	K	NIST Webbook
tb	364.70 ± 2.00	K	NIST Webbook
tc	539.07	K	Joback Method
tf	173.11	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.45	J/mol×K	362.02	Joback Method
cpg	153.14	J/mol×K	391.53	Joback Method
cpg	161.50	J/mol×K	421.04	Joback Method
cpg	169.54	J/mol×K	450.54	Joback Method
cpg	177.25	J/mol×K	480.05	Joback Method
cpg	184.66	J/mol×K	509.56	Joback Method
cpg	191.76	J/mol×K	539.07	Joback Method

dvisc	0.0063146	Pa×s	173.11	Joback Method
dvisc	0.0025690	Pa×s	204.59	Joback Method
dvisc	0.0013285	Pa×s	236.08	Joback Method
dvisc	0.0008023	Pa×s	267.56	Joback Method
dvisc	0.0005388	Pa×s	299.05	Joback Method
dvisc	0.0003904	Pa×s	330.53	Joback Method
dvisc	0.0002992	Pa×s	362.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1730978&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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