2,3-methylbutanoic acid

Other names: 2,3-dimethylbutyric acid
Inchi: InChI=1S/C6H12O2/c1-4(2)5(3)6(7)8/h4-5H,1-3H3,(H,7,8)
InchiKey: XFOASZQZPWEJAA-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CC(C)C(C)C(=O)O
Mol. weight [g/mol]: 116.16
CAS: 14287-61-7

Physical Properties

Property code	Value	Unit	Source
gf	-270.98	kJ/mol	Joback Method
hf	-442.54	kJ/mol	Joback Method
hfus	9.94	kJ/mol	Joback Method
hvap	51.60	kJ/mol	Joback Method
log10ws	-0.95		Crippen Method
logp	1.363		Crippen Method
mcvol	102.840	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	874.00		NIST Webbook
tb	481.85	K	Joback Method
tc	660.43	K	Joback Method
tf	271.60 ± 0.80	K	NIST Webbook
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.06	J/mol×K	481.85	Joback Method
cpg	233.51	J/mol×K	511.61	Joback Method
cpg	242.55	J/mol×K	541.38	Joback Method
cpg	251.20	J/mol×K	571.14	Joback Method
cpg	259.46	J/mol×K	600.90	Joback Method
cpg	267.34	J/mol×K	630.66	Joback Method
cpg	274.86	J/mol×K	660.43	Joback Method

dvisc	0.0917970	Pa×s	238.13	Joback Method
dvisc	0.0154044	Pa×s	278.75	Joback Method
dvisc	0.0040705	Pa×s	319.37	Joback Method
dvisc	0.0014524	Pa×s	359.99	Joback Method
dvisc	0.0006387	Pa×s	400.61	Joback Method
dvisc	0.0003267	Pa×s	441.23	Joback Method
dvisc	0.0001871	Pa×s	481.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14287617&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume