

4-Acetylbutyric acid

Other names:	5-Oxohexanoic acid 5-Ketohexanoic acid Hexanoic acid, 5-oxo- «delta»-Ketocaproic acid «delta»-Oxocaproic acid «gamma»-Acetylbutyric acid 5-Ketocaproic acid
Inchi:	InChI=1S/C6H10O3/c1-5(7)3-2-4-6(8)9/h2-4H2,1H3,(H,8,9)
InchiKey:	MGTZCLMLSSAXLD-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC(=O)CCCC(=O)O
Mol. weight [g/mol]:	130.14
CAS:	3128-06-1

Physical Properties

Property code	Value	Unit	Source
gf	-395.02	kJ/mol	Joback Method
hf	-544.56	kJ/mol	Joback Method
hfus	18.58	kJ/mol	Joback Method
hvap	59.12	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.830		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
tb	547.70	K	NIST Webbook
tc	717.02	K	Joback Method
tf	318.06	K	Joback Method
vc	0.403	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.46	J/mol×K	536.60	Joback Method
cpg	273.85	J/mol×K	686.95	Joback Method

cpg	267.09	J/molxK	656.88	Joback Method
cpg	259.98	J/molxK	626.81	Joback Method
cpg	252.51	J/molxK	596.74	Joback Method
cpg	244.67	J/molxK	566.67	Joback Method
cpg	280.28	J/molxK	717.02	Joback Method
dvisc	0.0001746	Paxs	536.60	Joback Method
dvisc	0.0002655	Paxs	500.18	Joback Method
dvisc	0.0004312	Paxs	463.75	Joback Method
dvisc	0.0007605	Paxs	427.33	Joback Method
dvisc	0.0014909	Paxs	390.91	Joback Method
dvisc	0.0033564	Paxs	354.48	Joback Method
dvisc	0.0090999	Paxs	318.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3128061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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