

3-Methyl-2-oxobutanoic acid

Inchi:	InChI=1S/C5H8O3/c1-3(2)4(6)5(7)8/h3H,1-2H3,(H,7,8)
InchiKey:	QHKABHOOEWYVLI-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	CC(C)C(=O)C(=O)O
Mol. weight [g/mol]:	116.12
CAS:	759-05-7

Physical Properties

Property code	Value	Unit	Source
af	0.6461		Cheméo Relay (1.0)
hf	-579.66	kJ/mol	Cheméo Relay (1.0)
hfus	16.93	kJ/mol	Joback Method
hvap	67.19	kJ/mol	Cheméo Relay (1.0)
ie	9.81	eV	Cheméo Relay (1.0)
log10ws	1.51e-04		Cheméo Relay (1.0)
logp	0.296		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
tb	454.37	K	Cheméo Relay (1.0)
tc	661.49	K	Cheméo Relay (1.0)
tf	304.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.343	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	8.62000e+00
Coeff. B	5.07540e-01
Coeff. C	-3.05300e-04

Coeff. D	6.67600e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.16264e+01
Coeff. B	1.83419e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	304.65
Temperature range (K), max.	502.96

Sources

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

McGowan Method:

https://en.wikipedia.org/wiki/Joback_method

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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