

acetoacetic acid

Inchi: InChI=1S/C4H6O3/c1-3(5)2-4(6)7/h2H2,1H3,(H,6,7)
InchiKey: WDJHALXBUFZDSR-UHFFFAOYSA-N
Formula: C4H6O3
SMILES: CC(=O)CC(=O)O
Mol. weight [g/mol]: 102.09
CAS: 541-50-4

Physical Properties

Property code	Value	Unit	Source
af	0.6346		Cheméo Relay (1.0)
gf	-490.03	kJ/mol	Joback Method
hf	-582.65	kJ/mol	Cheméo Relay (1.0)
hfus	17.86	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	0.64		Cheméo Relay (1.0)
logp	0.050		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	477.64	K	Cheméo Relay (1.0)
tc	699.16	K	Cheméo Relay (1.0)
tf	309.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.281	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	1.12110e+01
Coeff. B	4.06620e-01

Coeff. C	-2.47700e-04
Coeff. D	5.53600e-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	-1.14222e+01
Coeff. B	1.70221e+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.	309.65
Temperature range (K), max.	486.11

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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

McGowan Method:

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

Crippen Method:

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

Crippen Method:

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

Legend

af: Acentric Factor
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
hvac:	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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