

2-acetoxypropanoic acid

Other names:	«alpha»-Acetoxypropionic acid
Inchi:	InChI=1S/C5H8O4/c1-3(5(7)8)9-4(2)6/h3H,1-2H3,(H,7,8)
InchiKey:	WTLNOANVTIKPEE-UHFFFAOYSA-N
Formula:	C5H8O4
SMILES:	CC(=O)OC(C)C(=O)O
Mol. weight [g/mol]:	132.11
CAS:	535-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-510.88	kJ/mol	Joback Method
hf	-661.42	kJ/mol	Joback Method
hfus	13.66	kJ/mol	Joback Method
hvap	58.92	kJ/mol	Joback Method
log10ws	0.01		Crippen Method
logp	0.023		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	4510.35	kPa	Joback Method
rinpol	1067.00		NIST Webbook
tb	535.70	K	Joback Method
tc	720.64	K	Joback Method
tf	331.50 ± 1.50	K	NIST Webbook
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.57	J/molxK	535.70	Joback Method
cpg	249.29	J/molxK	689.82	Joback Method
cpg	243.16	J/molxK	658.99	Joback Method
cpg	236.72	J/molxK	628.17	Joback Method
cpg	229.98	J/molxK	597.35	Joback Method
cpg	222.93	J/molxK	566.52	Joback Method
cpg	255.10	J/molxK	720.64	Joback Method

dvisc	0.0001468	Paxs	535.70	Joback Method
dvisc	0.0002271	Paxs	498.75	Joback Method
dvisc	0.0003765	Paxs	461.81	Joback Method
dvisc	0.0006818	Paxs	424.86	Joback Method
dvisc	0.0013824	Paxs	387.91	Joback Method
dvisc	0.0032528	Paxs	350.97	Joback Method
dvisc	0.0093612	Paxs	314.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.00	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C535171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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