

Acetic acid-d4

Other names:	[2H3]acetic [2H]acid ethanoic acid-d4
Inchi:	InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4)/i1D3/hD
InchiKey:	QTBSBXVTEAMEQO-GUEYOVJQSA-N
Formula:	C2D4O2
SMILES:	CC(=O)O
Mol. weight [g/mol]:	64.08
CAS:	1186-52-3

Physical Properties

Property code	Value	Unit	Source
gf	-299.78	kJ/mol	Joback Method
hf	-349.42	kJ/mol	Joback Method
hfus	6.62	kJ/mol	Joback Method
hvap	43.47	kJ/mol	Joback Method
log10ws	0.24		Crippen Method
logp	0.091		Crippen Method
mvol	46.480	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
tb	391.21	K	Joback Method
tc	567.09	K	Joback Method
tf	223.05	K	Joback Method
vc	0.172	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	77.89	J/molxK	391.21	Joback Method
cpg	81.64	J/molxK	420.52	Joback Method
cpg	85.25	J/molxK	449.84	Joback Method
cpg	88.73	J/molxK	479.15	Joback Method
cpg	92.08	J/molxK	508.46	Joback Method
cpg	95.29	J/molxK	537.78	Joback Method
cpg	98.37	J/molxK	567.09	Joback Method

dvisc	0.0414396	Paxs	223.05	Joback Method
dvisc	0.0120716	Paxs	251.08	Joback Method
dvisc	0.0045049	Paxs	279.10	Joback Method
dvisc	0.0020125	Paxs	307.13	Joback Method
dvisc	0.0010288	Paxs	335.16	Joback Method
dvisc	0.0005833	Paxs	363.18	Joback Method
dvisc	0.0003587	Paxs	391.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1186523&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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