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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0414396	Pa×s	223.05	Joback Method
dvisc	0.0120716	Pa×s	251.08	Joback Method
dvisc	0.0045049	Pa×s	279.10	Joback Method
dvisc	0.0020125	Pa×s	307.13	Joback Method
dvisc	0.0010288	Pa×s	335.16	Joback Method
dvisc	0.0005833	Pa×s	363.18	Joback Method
dvisc	0.0003587	Pa×s	391.21	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=C1186523&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume