3-Butynoic acid

Other names:	CH«equiv»CCH2COOH
	but-3-ynoic acid
Inchi:	InChI=1S/C4H4O2/c1-2-3-4(5)6/h1H,3H2,(H,5,6)
InchiKey:	KKAHGSQLSTUDAV-UHFFFAOYSA-N
Formula:	C4H4O2
SMILES:	C#CCC(=O)O
Mol. weight [g/mol]:	84.07
CAS:	2345-51-9

Physical Properties

Property code	Value	Unit	Source
gf	-59.87	kJ/mol	Joback Method
hf	-98.80	kJ/mol	Joback Method
hfus	14.78	kJ/mol	Joback Method
hvap	47.78	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.094		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	5926.27	kPa	Joback Method
tb	427.09	K	Joback Method
tc	613.16	K	Joback Method
tf	292.56	K	Joback Method
vc	0.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.64	J/mol×K	427.09	Joback Method
cpg	124.30	J/mol×K	458.10	Joback Method
cpg	128.72	J/mol×K	489.11	Joback Method
cpg	132.91	J/mol×K	520.13	Joback Method
cpg	136.88	J/mol×K	551.14	Joback Method
cpg	140.63	J/mol×K	582.15	Joback Method
cpg	144.19	J/mol×K	613.16	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=C2345519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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