

2-Butynedioic acid

Other names:	Acetylenedicarboxylic acid Butynedioic acid
Inchi:	InChI=1S/C4H2O4/c5-3(6)1-2-4(7)8/h(H,5,6)(H,7,8)
InchiKey:	YTIVTFGABIZHHX-UHFFFAOYSA-N
Formula:	C4H2O4
SMILES:	O=C(O)C#CC(=O)O
Mol. weight [g/mol]:	114.06
CAS:	142-45-0

Physical Properties

Property code	Value	Unit	Source
gf	-345.88	kJ/mol	Joback Method
hf	-383.21	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	73.50	kJ/mol	Joback Method
log10ws	0.51		Crippen Method
logp	-0.841		Crippen Method
mvol	73.500	ml/mol	McGowan Method
pc	7803.82	kPa	Joback Method
tb	592.02	K	Joback Method
tc	787.12	K	Joback Method
tf	439.65 ± 2.50	K	NIST Webbook
vc	0.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.42	J/mol×K	592.02	Joback Method
cpg	151.08	J/mol×K	624.54	Joback Method
cpg	154.55	J/mol×K	657.05	Joback Method
cpg	157.82	J/mol×K	689.57	Joback Method
cpg	160.90	J/mol×K	722.08	Joback Method
cpg	163.79	J/mol×K	754.60	Joback Method
cpg	166.50	J/mol×K	787.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C142450&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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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