4-Pentynoic acid

Other names: Pent-4-yn-1-oic acid
Propargylacetic acid
pent-4-ynoic acid
Inchi: InChI=1S/C5H6O2/c1-2-3-4-5(6)7/h1H,3-4H2,(H,6,7)
InchiKey: MLBYLEUJXUBIJJ-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: C#CCCC(=O)O
Mol. weight [g/mol]: 98.10
CAS: 6089-09-4

Physical Properties

Property code	Value	Unit	Source
gf	-51.45	kJ/mol	Joback Method
hf	-119.44	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-0.81		Crippen Method
logp	0.484		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	5138.68	kPa	Joback Method
tb	449.97	K	Joback Method
tc	634.40	K	Joback Method
tf	329.00 ± 3.00	K	NIST Webbook
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.01	J/mol×K	449.97	Joback Method
cpg	161.06	J/mol×K	480.71	Joback Method
cpg	166.80	J/mol×K	511.45	Joback Method
cpg	172.26	J/mol×K	542.18	Joback Method
cpg	177.44	J/mol×K	572.92	Joback Method
cpg	182.35	J/mol×K	603.66	Joback Method

cpg	187.02	J/mol×K	634.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	4.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6089094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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