3-methyl-3-pentenoic acid

Inchi: InChI=1S/C6H10O2/c1-3-5(2)4-6(7)8/h3H,4H2,1-2H3,(H,7,8)/b5-3+
InchiKey: OGVROELYPSGUQB-HWKANZROSA-N
Formula: C6H10O2
SMILES: CC=C(C)CC(=O)O
Mol. weight [g/mol]: 114.14

Physical Properties

Property code	Value	Unit	Source
gf	-194.43	kJ/mol	Joback Method
hf	-324.55	kJ/mol	Joback Method
hfus	15.88	kJ/mol	Joback Method
hvap	52.41	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.427		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
ripol	1982.00		NIST Webbook
ripol	1982.00		NIST Webbook
tb	486.77	K	Joback Method
tc	669.02	K	Joback Method
tf	249.09	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.98	J/mol×K	486.77	Joback Method
cpg	214.52	J/mol×K	517.15	Joback Method
cpg	222.63	J/mol×K	547.52	Joback Method
cpg	230.34	J/mol×K	577.90	Joback Method
cpg	237.66	J/mol×K	608.27	Joback Method
cpg	244.62	J/mol×K	638.65	Joback Method
cpg	251.22	J/mol×K	669.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R335025&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume