(E)-2-Methyl-2-butenoic acid

Inchi: InChI=1S/C5H8O2/c1-3-4(2)5(6)7/h3H,1-2H3,(H,6,7)/b4-3+
InchiKey: UIERETOOQGIECD-ONEGZZNKSA-N
Formula: C5H8O2
SMILES: CC=C(C)C(=O)O
Mol. weight [g/mol]: 100.12

Physical Properties

Property code	Value	Unit	Source
gf	-202.85	kJ/mol	Joback Method
hf	-303.91	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	50.19	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	1.037		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
rinpol	941.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1862.00		NIST Webbook
ripol	1867.00		NIST Webbook
tb	463.89	K	Joback Method
tc	647.95	K	Joback Method
tf	237.82	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.62	J/mol×K	463.89	Joback Method
cpg	174.00	J/mol×K	494.57	Joback Method
cpg	181.01	J/mol×K	525.24	Joback Method
cpg	187.67	J/mol×K	555.92	Joback Method
cpg	193.97	J/mol×K	586.60	Joback Method
cpg	199.96	J/mol×K	617.27	Joback Method

cpg	205.63	J/mol×K	647.95	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=R604470&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume