2-Methyl-2-propenoic acid

Inchi: InChI=1S/C8H12O2/c1-6(2)5-10-8(9)7(3)4/h1,3,5H2,2,4H3
InchiKey: TVBLIEXOPWWREN-UHFFFAOYSA-N
Formula: C8H12O2
SMILES: C=C(C)COC(=O)C(=C)C
Mol. weight [g/mol]: 140.18
CAS: 816-74-0

Physical Properties

Property code	Value	Unit	Source
gf	-58.86	kJ/mol	Joback Method
hf	-221.97	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	41.38	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.682		Crippen Method
mcvol	122.420	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
rinpol	954.00		NIST Webbook
rinpol	954.00		NIST Webbook
tb	451.85	K	Joback Method
tc	641.06	K	Joback Method
tf	220.64	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.48	J/mol×K	451.85	Joback Method
cpg	257.84	J/mol×K	483.38	Joback Method
cpg	268.71	J/mol×K	514.92	Joback Method
cpg	279.10	J/mol×K	546.45	Joback Method
cpg	289.02	J/mol×K	577.99	Joback Method
cpg	298.48	J/mol×K	609.52	Joback Method
cpg	307.49	J/mol×K	641.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C816740&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume