2-Allyl-4-methyl-4-pentenoic acid

Inchi: InChI=1S/C9H14O2/c1-4-5-8(9(10)11)6-7(2)3/h4,8H,1-2,5-6H2,3H3,(H,10,11)
InchiKey: LLWNYXLAJUISMK-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: C=CCC(CC(=C)C)C(=O)O
Mol. weight [g/mol]: 154.21
CAS: 93681-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-76.15	kJ/mol	Joback Method
hf	-258.11	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	2.229		Crippen Method
mcvol	136.510	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	544.17	K	Joback Method
tc	723.79	K	Joback Method
tf	269.46	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.80	J/mol×K	544.17	Joback Method
cpg	327.70	J/mol×K	574.11	Joback Method
cpg	338.05	J/mol×K	604.04	Joback Method
cpg	347.89	J/mol×K	633.98	Joback Method
cpg	357.23	J/mol×K	663.92	Joback Method
cpg	366.10	J/mol×K	693.85	Joback Method
cpg	374.51	J/mol×K	723.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93681824&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume