2-Butenoic acid, 2,3-dimethyl-

Inchi: InChI=1S/C6H10O2/c1-4(2)5(3)6(7)8/h1-3H3,(H,7,8)
InchiKey: UAXOELSVPTZZQG-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CC(C)=C(C)C(=O)O
Mol. weight [g/mol]: 114.14
CAS: 4411-97-6

Physical Properties

Property code	Value	Unit	Source
gf	-202.98	kJ/mol	Joback Method
hf	-334.34	kJ/mol	Joback Method
hfus	14.57	kJ/mol	Joback Method
hvap	52.49	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.427		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	486.65	K	Joback Method
tc	672.20	K	Joback Method
tf	235.13	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.88	J/mol×K	486.65	Joback Method
cpg	214.54	J/mol×K	517.58	Joback Method
cpg	222.76	J/mol×K	548.50	Joback Method
cpg	230.56	J/mol×K	579.43	Joback Method
cpg	237.96	J/mol×K	610.35	Joback Method
cpg	244.99	J/mol×K	641.28	Joback Method
cpg	251.66	J/mol×K	672.20	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=C4411976&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume