(E) Methyl 2-chloro-3-methoxy-2-butenoate

Inchi: InChI=1S/C6H9ClO3/c1-4(9-2)5(7)6(8)10-3/h1-3H3/b5-4+
InchiKey: UCQQBIORXJIZBS-SNAWJCMRSA-N
Formula: C6H9ClO3
SMILES: COC(=O)C(Cl)=C(C)OC
Mol. weight [g/mol]: 164.59
CAS: 82481-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-288.09	kJ/mol	Joback Method
hf	-462.29	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	45.02	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.276		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	476.74	K	Joback Method
tc	676.44	K	Joback Method
tf	248.69	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.15	J/mol×K	476.74	Joback Method
cpg	238.42	J/mol×K	510.02	Joback Method
cpg	247.33	J/mol×K	543.31	Joback Method
cpg	255.86	J/mol×K	576.59	Joback Method
cpg	264.02	J/mol×K	609.87	Joback Method
cpg	271.81	J/mol×K	643.15	Joback Method
cpg	279.23	J/mol×K	676.44	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=C82481241&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