3-Penten-2-one, 3-chloro-4-methoxy-, (Z)-

Inchi: InChI=1S/C6H9ClO2/c1-4(8)6(7)5(2)9-3/h1-3H3/b6-5-
InchiKey: HFVPSGDRPXDAAV-WAYWQWQTSA-N
Formula: C6H9ClO2
SMILES: COC(C)=C(Cl)C(C)=O
Mol. weight [g/mol]: 148.59
CAS: 66694-88-0

Physical Properties

Property code	Value	Unit	Source
gf	-183.09	kJ/mol	Joback Method
hf	-330.07	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	42.61	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.692		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3368.44	kPa	Joback Method
tb	454.32	K	Joback Method
tc	655.34	K	Joback Method
tf	226.46	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.13	J/mol×K	454.32	Joback Method
cpg	217.56	J/mol×K	487.82	Joback Method
cpg	226.54	J/mol×K	521.33	Joback Method
cpg	235.08	J/mol×K	554.83	Joback Method
cpg	243.21	J/mol×K	588.34	Joback Method
cpg	250.92	J/mol×K	621.84	Joback Method
cpg	258.24	J/mol×K	655.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66694880&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