Methyl 2,3-dichloro-4-oxopentenoate

Inchi: InChI=1S/C6H8Cl2O3/c1-3(9)4(7)5(8)6(10)11-2/h4-5H,1-2H3
InchiKey: GOJJJWQYCJZBOM-UHFFFAOYSA-N
Formula: C6H8Cl2O3
SMILES: COC(=O)C(Cl)C(Cl)C(C)=O
Mol. weight [g/mol]: 199.03

Physical Properties

Property code	Value	Unit	Source
gf	-391.94	kJ/mol	Joback Method
hf	-566.59	kJ/mol	Joback Method
hfus	17.03	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	0.963		Crippen Method
mcvol	128.890	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1158.00		NIST Webbook
tb	540.82	K	Joback Method
tc	748.93	K	Joback Method
tf	309.31	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.46	J/mol×K	540.82	Joback Method
cpg	301.77	J/mol×K	714.24	Joback Method
cpg	294.63	J/mol×K	679.56	Joback Method
cpg	287.04	J/mol×K	644.87	Joback Method
cpg	278.98	J/mol×K	610.19	Joback Method
cpg	270.45	J/mol×K	575.50	Joback Method
cpg	308.44	J/mol×K	748.93	Joback Method
dvisc	0.0002864	Pa×s	540.82	Joback Method
dvisc	0.0003755	Pa×s	502.23	Joback Method

dvisc	0.0005152	Pa×s	463.65	Joback Method
dvisc	0.0007485	Pa×s	425.06	Joback Method
dvisc	0.0011717	Pa×s	386.48	Joback Method
dvisc	0.0020260	Pa×s	347.89	Joback Method
dvisc	0.0040160	Pa×s	309.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R80376&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
dvisc:	Dynamic viscosity
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