Dimethyl chlorobutenedioate

Inchi: InChI=1S/C6H7ClO4/c1-10-5(8)3-4(7)6(9)11-2/h3H,1-2H3/b4-3-
InchiKey: VYXGXXYXSAMWBM-ARJAWSKDSA-N
Formula: C6H7ClO4
SMILES: COC(=O)C=C(Cl)C(=O)OC
Mol. weight [g/mol]: 178.57

Physical Properties

Property code	Value	Unit	Source
gf	-408.46	kJ/mol	Joback Method
hf	-565.08	kJ/mol	Joback Method
hfus	19.96	kJ/mol	Joback Method
hvap	51.69	kJ/mol	Joback Method
log10ws	-0.56		Crippen Method
logp	0.455		Crippen Method
mcvol	118.220	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1068.00		NIST Webbook
rinpol	1094.00		NIST Webbook
tb	530.73	K	Joback Method
tc	736.15	K	Joback Method
tf	312.58	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.54	J/mol×K	530.73	Joback Method
cpg	248.95	J/mol×K	564.97	Joback Method
cpg	256.98	J/mol×K	599.20	Joback Method
cpg	264.61	J/mol×K	633.44	Joback Method
cpg	271.86	J/mol×K	667.68	Joback Method
cpg	278.70	J/mol×K	701.91	Joback Method
cpg	285.16	J/mol×K	736.15	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=R80166&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume