Dimethyl 2,3-dichlorobutenedioate

Inchi: InChI=1S/C6H6Cl2O4/c1-11-5(9)3(7)4(8)6(10)12-2/h1-2H3/b4-3+
InchiKey: YGDFORZEKOJPAN-ONEGZZNKSA-N
Formula: C6H6Cl2O4
SMILES: COC(=O)C(Cl)=C(Cl)C(=O)OC
Mol. weight [g/mol]: 213.01

Physical Properties

Property code	Value	Unit	Source
gf	-428.94	kJ/mol	Joback Method
hf	-590.61	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	56.15	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.022		Crippen Method
mcvol	130.460	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1216.00		NIST Webbook
tb	568.04	K	Joback Method
tc	781.75	K	Joback Method
tf	328.54	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.35	J/mol×K	568.04	Joback Method
cpg	269.34	J/mol×K	603.66	Joback Method
cpg	276.90	J/mol×K	639.28	Joback Method
cpg	284.03	J/mol×K	674.89	Joback Method
cpg	290.74	J/mol×K	710.51	Joback Method
cpg	297.01	J/mol×K	746.13	Joback Method
cpg	302.86	J/mol×K	781.75	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R80148&Units=SI

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