Dimethyl 2-chloro-4-bromo-3-oxopentanedioate

Inchi: InChI=1S/C6H6BrClO3/c1-3(7)5(9)4(8)6(10)11-2/h4H,1H2,2H3
InchiKey: SAGQKOKUIJJBAB-UHFFFAOYSA-N
Formula: C6H6BrClO3
SMILES: C=C(Br)C(=O)C(Cl)C(=O)OC
Mol. weight [g/mol]: 241.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.96	kJ/mol	Joback Method
hf	-403.60	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	54.69	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.244		Crippen Method
mcvol	129.850	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	566.55	K	Joback Method
tc	787.74	K	Joback Method
tf	338.47	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.24	J/mol×K	566.55	Joback Method
cpg	258.16	J/mol×K	603.41	Joback Method
cpg	265.58	J/mol×K	640.28	Joback Method
cpg	272.50	J/mol×K	677.14	Joback Method
cpg	278.95	J/mol×K	714.01	Joback Method
cpg	284.94	J/mol×K	750.87	Joback Method
cpg	290.49	J/mol×K	787.74	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=R80273&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