

Methyl 4,5-dibromo-2-chloro-3-oxopentanoate

Inchi:	InChI=1S/C6H7Br2ClO3/c1-12-6(11)4(9)5(10)3(8)2-7/h3-4H,2H2,1H3
InchiKey:	VQMVZGZYYJCLJS-UHFFFAOYSA-N
Formula:	C6H7Br2ClO3
SMILES:	COC(=O)C(Cl)C(=O)C(Br)CBr
Mol. weight [g/mol]:	322.38

Physical Properties

Property code	Value	Unit	Source
gf	-351.37	kJ/mol	Joback Method
hf	-498.19	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	61.33	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.494		Crippen Method
mcvol	151.650	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
rinpola	1528.00		NIST Webbook
tb	635.71	K	Joback Method
tc	865.44	K	Joback Method
tf	398.99	K	Joback Method
vc	0.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.42	J/molxK	635.71	Joback Method
cpg	332.59	J/molxK	827.15	Joback Method
cpg	326.82	J/molxK	788.86	Joback Method
cpg	320.53	J/molxK	750.57	Joback Method
cpg	313.72	J/molxK	712.29	Joback Method
cpg	306.36	J/molxK	674.00	Joback Method
cpg	337.88	J/molxK	865.44	Joback Method
dvisc	0.0002440	Paxs	635.71	Joback Method
dvisc	0.0003102	Paxs	596.26	Joback Method

dvisc	0.0004081	Paxs	556.80	Joback Method
dvisc	0.0005597	Paxs	517.35	Joback Method
dvisc	0.0008087	Paxs	477.90	Joback Method
dvisc	0.0012484	Paxs	438.44	Joback Method
dvisc	0.0021003	Paxs	398.99	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=R80401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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