

Methyl 2,4-dichloro-2-bromo-3-oxobutanoate

Inchi:	InChI=1S/C5H5BrCl2O3/c1-11-4(10)5(6,8)3(9)2-7/h2H2,1H3
InchiKey:	VQUPDNAUQJHMIG-UHFFFAOYSA-N
Formula:	C5H5BrCl2O3
SMILES:	COC(=O)C(Cl)(Br)C(=O)CCl
Mol. weight [g/mol]:	263.90

Physical Properties

Property code	Value	Unit	Source
gf	-378.32	kJ/mol	Joback Method
hf	-517.81	kJ/mol	Joback Method
hfus	19.36	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.297		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1328.00		NIST Webbook
tb	581.75	K	Joback Method
tc	811.21	K	Joback Method
tf	390.26	K	Joback Method
vc	0.494	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.27	J/mol×K	581.75	Joback Method
cpg	257.30	J/mol×K	619.99	Joback Method
cpg	263.74	J/mol×K	658.24	Joback Method
cpg	269.64	J/mol×K	696.48	Joback Method
cpg	275.02	J/mol×K	734.72	Joback Method
cpg	279.92	J/mol×K	772.97	Joback Method
cpg	284.37	J/mol×K	811.21	Joback Method
dvisc	0.0020519	Paxs	390.26	Joback Method

dvisc	0.0013235	Paxs	422.18	Joback Method
dvisc	0.0009079	Paxs	454.09	Joback Method
dvisc	0.0006545	Paxs	486.00	Joback Method
dvisc	0.0004912	Paxs	517.92	Joback Method
dvisc	0.0003811	Paxs	549.84	Joback Method
dvisc	0.0003041	Paxs	581.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R80380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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