Acetic acid, bromochloro-, methyl ester

Other names: Methyl bromochloroacetate
Inchi: InChI=1S/C3H4BrClO2/c1-7-3(6)2(4)5/h2H,1H3
InchiKey: WIBYPHGWXYLWQX-UHFFFAOYSA-N
Formula: C3H4BrClO2
SMILES: COC(=O)C(Cl)Br
Mol. weight [g/mol]: 187.42
CAS: 20428-74-4

Physical Properties

Property code	Value	Unit	Source
gf	-259.59	kJ/mol	Joback Method
hf	-344.74	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	41.86	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.119		Crippen Method
mcvol	90.310	ml/mol	McGowan Method
pc	4959.33	kPa	Joback Method
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
tb	447.48	K	Joback Method
tc	660.61	K	Joback Method
tf	270.45	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.95	J/mol×K	447.48	Joback Method
cpg	148.40	J/mol×K	483.00	Joback Method
cpg	153.59	J/mol×K	518.52	Joback Method
cpg	158.53	J/mol×K	554.04	Joback Method
cpg	163.21	J/mol×K	589.56	Joback Method
cpg	167.65	J/mol×K	625.08	Joback Method

cpg	171.84	J/mol×K	660.61	Joback Method
dvisc	0.0033184	Pa×s	270.45	Joback Method
dvisc	0.0019547	Pa×s	299.95	Joback Method
dvisc	0.0012659	Pa×s	329.46	Joback Method
dvisc	0.0008805	Pa×s	358.97	Joback Method
dvisc	0.0006472	Pa×s	388.47	Joback Method
dvisc	0.0004968	Pa×s	417.98	Joback Method
dvisc	0.0003949	Pa×s	447.48	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=C20428744&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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