

Methyl 3-bromo-2-(bromomethyl)propionate

Other names:	Propanoic acid, 3-bromo-2-(bromomethyl)-, methyl ester
Inchi:	InChI=1S/C5H8Br2O2/c1-9-5(8)4(2-6)3-7/h4H,2-3H2,1H3
InchiKey:	USXVPPOARMSYGY-UHFFFAOYSA-N
Formula:	C5H8Br2O2
SMILES:	COC(=O)C(CBr)CBr
Mol. weight [g/mol]:	259.92
CAS:	22262-60-8

Physical Properties

Property code	Value	Unit	Source
gf	-216.50	kJ/mol	Joback Method
hf	-343.95	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	1.565		Crippen Method
mcvol	123.750	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	521.97	K	Joback Method
tc	739.28	K	Joback Method
tf	322.87	K	Joback Method
vc	0.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.54	J/molxK	521.97	Joback Method
cpg	234.87	J/molxK	558.19	Joback Method
cpg	242.73	J/molxK	594.41	Joback Method
cpg	250.14	J/molxK	630.63	Joback Method
cpg	257.11	J/molxK	666.84	Joback Method
cpg	263.67	J/molxK	703.06	Joback Method
cpg	269.82	J/molxK	739.28	Joback Method
dvisc	0.0026265	Paxs	322.87	Joback Method

dvisc	0.0015817	Paxs	356.05	Joback Method
dvisc	0.0010386	Paxs	389.24	Joback Method
dvisc	0.0007285	Paxs	422.42	Joback Method
dvisc	0.0005381	Paxs	455.60	Joback Method
dvisc	0.0004142	Paxs	488.79	Joback Method
dvisc	0.0003296	Paxs	521.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	334.20	K	0.05	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22262608&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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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