

Methyl 2-bromobutanoate

Inchi:	InChI=1S/C5H9BrO2/c1-3-4(6)5(7)8-2/h4H,3H2,1-2H3
InchiKey:	UFQQDNMQADCHGH-UHFFFAOYSA-N
Formula:	C5H9BrO2
SMILES:	CCC(Br)C(=O)OC
Mol. weight [g/mol]:	181.03
CAS:	69043-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-230.82	kJ/mol	Joback Method
hf	-370.28	kJ/mol	Joback Method
hfus	13.25	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.333		Crippen Method
mcvol	106.250	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
rinpol	926.00		NIST Webbook
tb	455.81	K	Joback Method
tc	657.09	K	Joback Method
tf	263.07	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.09	J/molxK	455.81	Joback Method
cpg	204.86	J/molxK	489.36	Joback Method
cpg	213.25	J/molxK	522.90	Joback Method
cpg	221.27	J/molxK	556.45	Joback Method
cpg	228.93	J/molxK	590.00	Joback Method
cpg	236.22	J/molxK	623.55	Joback Method
cpg	243.15	J/molxK	657.09	Joback Method
dvisc	0.0035835	Paxs	263.07	Joback Method

dvisc	0.0019491	Paxs	295.19	Joback Method
dvisc	0.0011948	Paxs	327.32	Joback Method
dvisc	0.0007993	Paxs	359.44	Joback Method
dvisc	0.0005712	Paxs	391.56	Joback Method
dvisc	0.0004295	Paxs	423.69	Joback Method
dvisc	0.0003362	Paxs	455.81	Joback Method

Sources

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=C69043965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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