

Isobutyl 2-bromobutanoate

Inchi:	InChI=1S/C8H15BrO2/c1-4-7(9)8(10)11-5-6(2)3/h6-7H,4-5H2,1-3H3
InchiKey:	FIUCVOFYLPFAI-UHFFFAOYSA-N
Formula:	C8H15BrO2
SMILES:	CCC(Br)C(=O)OCC(C)C
Mol. weight [g/mol]:	223.11

Physical Properties

Property code	Value	Unit	Source
gf	-208.00	kJ/mol	Joback Method
hf	-437.48	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	48.22	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.359		Crippen Method
mcvol	148.520	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rmpol	1144.00		NIST Webbook
tb	524.01	K	Joback Method
tc	721.87	K	Joback Method
tf	281.88	K	Joback Method
vc	0.557	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.93	J/molxK	524.01	Joback Method
cpg	333.49	J/molxK	556.99	Joback Method
cpg	345.46	J/molxK	589.96	Joback Method
cpg	356.85	J/molxK	622.94	Joback Method
cpg	367.67	J/molxK	655.92	Joback Method
cpg	377.94	J/molxK	688.90	Joback Method
cpg	387.67	J/molxK	721.87	Joback Method
dvisc	0.0045596	Paxs	281.88	Joback Method
dvisc	0.0020562	Paxs	322.24	Joback Method

dvisc	0.0011072	Paxs	362.59	Joback Method
dvisc	0.0006748	Paxs	402.94	Joback Method
dvisc	0.0004501	Paxs	443.30	Joback Method
dvisc	0.0003212	Paxs	483.65	Joback Method
dvisc	0.0002415	Paxs	524.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R23447&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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