

Isobutyryl bromide

Other names:	Propanoyl bromide, 2-methyl-
Inchi:	InChI=1S/C4H7BrO/c1-3(2)4(5)6/h3H,1-2H3
InchiKey:	ICNCZFQYZKPYMS-UHFFFAOYSA-N
Formula:	C4H7BrO
SMILES:	CC(C)C(=O)Br
Mol. weight [g/mol]:	151.00
CAS:	2736-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-134.24	kJ/mol	Joback Method
hf	-217.42	kJ/mol	Joback Method
hfus	9.48	kJ/mol	Joback Method
hvap	37.29	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.564		Crippen Method
mcvol	86.290	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	388.00 ± 3.00	K	NIST Webbook
tc	615.14	K	Joback Method
tf	229.57	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.84	J/mol×K	615.14	Joback Method
cpg	139.44	J/mol×K	410.51	Joback Method
cpg	146.94	J/mol×K	444.61	Joback Method
cpg	154.04	J/mol×K	478.72	Joback Method
cpg	160.77	J/mol×K	512.82	Joback Method
cpg	167.14	J/mol×K	546.93	Joback Method
cpg	173.16	J/mol×K	581.03	Joback Method
dvisc	0.0004246	Pa×s	410.51	Joback Method

dvisc	0.0047331	Pa×s	229.57	Joback Method
dvisc	0.0025078	Pa×s	259.73	Joback Method
dvisc	0.0015165	Pa×s	289.88	Joback Method
dvisc	0.0010082	Pa×s	320.04	Joback Method
dvisc	0.0007191	Pa×s	350.20	Joback Method
dvisc	0.0005411	Pa×s	380.35	Joback Method
hvapt	45.70	kJ/mol	361.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2736370&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvapt:	Enthalpy of vaporization at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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