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

Physical Properties

Property code	Value	Unit	Source
af	0.3776		Cheméo Relay (1.0)
hf	-228.05	kJ/mol	Cheméo Relay (1.0)
hfus	9.48	kJ/mol	Joback Method
hvap	33.22	kJ/mol	Cheméo Relay (1.0)
ie	10.04	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
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	569.98	K	Cheméo Relay (1.0)
tf	188.39	K	Cheméo Relay (1.0)
vc	0.318	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.44	J/mol×K	410.51	Joback Method
cpg	178.84	J/mol×K	615.14	Joback Method
cpg	173.16	J/mol×K	581.03	Joback Method
cpg	167.14	J/mol×K	546.93	Joback Method
cpg	160.77	J/mol×K	512.82	Joback Method
cpg	154.04	J/mol×K	478.72	Joback Method
cpg	146.94	J/mol×K	444.61	Joback Method
dvisc	0.0010082	Pa×s	320.04	Joback Method

dvisc	0.0004246	Pa×s	410.51	Joback Method
dvisc	0.0005411	Pa×s	380.35	Joback Method
dvisc	0.0007191	Pa×s	350.20	Joback Method
dvisc	0.0047331	Pa×s	229.57	Joback Method
dvisc	0.0015165	Pa×s	289.88	Joback Method
dvisc	0.0025078	Pa×s	259.73	Joback Method
hvapt	45.70	kJ/mol	361.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2736370&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
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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