Propanoyl bromide, 2-bromo-2-methyl-

Other names:	2-Bromoisobutyryl bromide
	«alpha»-Bromoisobutyryl bromide
	2-Bromo-2-methyl-propionyl bromide
Inchi:	InChI=1S/C4H6Br2O/c1-4(2,6)3(5)7/h1-2H3
InchiKey:	YOCIJWAHRAJQFT-UHFFFAOYSA-N
Formula:	C4H6Br2O
SMILES:	CC(C)(Br)C(=O)Br
Mol. weight [g/mol]:	229.90
CAS:	20769-85-1

Physical Properties

Property code	Value	Unit	Source
gf	-114.64	kJ/mol	Joback Method
hf	-194.56	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	42.82	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.081		Crippen Method
mcvol	103.790	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	436.20	K	NIST Webbook
tc	707.16	K	Joback Method
tf	306.79	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.82	J/mol×K	473.88	Joback Method
cpg	178.48	J/mol×K	512.76	Joback Method
cpg	185.45	J/mol×K	551.64	Joback Method
cpg	191.77	J/mol×K	590.52	Joback Method
cpg	197.51	J/mol×K	629.40	Joback Method
cpg	202.73	J/mol×K	668.28	Joback Method

cpg	207.48	J/mol×K	707.16	Joback Method
dvisc	0.0035573	Pa×s	306.79	Joback Method
dvisc	0.0022169	Pa×s	334.64	Joback Method
dvisc	0.0014857	Pa×s	362.49	Joback Method
dvisc	0.0010542	Pa×s	390.34	Joback Method
dvisc	0.0007829	Pa×s	418.18	Joback Method
dvisc	0.0006035	Pa×s	446.03	Joback Method
dvisc	0.0004797	Pa×s	473.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.70	K	13.30	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20769851&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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