

5-Bromopentanoyl chloride

Inchi:	InChI=1S/C5H8BrClO/c6-4-2-1-3-5(7)8/h1-4H2
InchiKey:	OKRUMSWHDWKGHA-UHFFFAOYSA-N
Formula:	C5H8BrClO
SMILES:	O=C(Cl)CCCCBr
Mol. weight [g/mol]:	199.47
CAS:	4509-90-4

Physical Properties

Property code	Value	Unit	Source
gf	-135.31	kJ/mol	Joback Method
hf	-248.52	kJ/mol	Joback Method
hfus	19.79	kJ/mol	Joback Method
hvap	44.29	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.317		Crippen Method
mcvol	112.620	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	471.26	K	Joback Method
tc	675.44	K	Joback Method
tf	285.76	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.70	J/molxK	471.26	Joback Method
cpg	205.90	J/molxK	505.29	Joback Method
cpg	213.64	J/molxK	539.32	Joback Method
cpg	220.95	J/molxK	573.35	Joback Method
cpg	227.85	J/molxK	607.38	Joback Method
cpg	234.34	J/molxK	641.41	Joback Method
cpg	240.46	J/molxK	675.44	Joback Method
dvisc	0.0033035	Paxs	285.76	Joback Method
dvisc	0.0019900	Paxs	316.68	Joback Method

dvisc	0.0013119	Paxs	347.59	Joback Method
dvisc	0.0009257	Paxs	378.51	Joback Method
dvisc	0.0006886	Paxs	409.43	Joback Method
dvisc	0.0005339	Paxs	440.34	Joback Method
dvisc	0.0004280	Paxs	471.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4509904&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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