

Hexanoyl chloride, 6-bromo-

Other names:	6-Bromohexanoyl chloride
Inchi:	InChI=1S/C6H10BrClO/c7-5-3-1-2-4-6(8)9/h1-5H2
InchiKey:	HBPVGJGGBRWIVSX-UHFFFAOYSA-N
Formula:	C6H10BrClO
SMILES:	O=C(Cl)CCCCCBr
Mol. weight [g/mol]:	213.50
CAS:	22809-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-126.89	kJ/mol	Joback Method
hf	-269.16	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	46.52	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.707		Crippen Method
mcvol	126.710	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	494.14	K	Joback Method
tc	695.58	K	Joback Method
tf	297.03	K	Joback Method
vc	0.488	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.45	J/molxK	494.14	Joback Method
cpg	279.68	J/molxK	662.01	Joback Method
cpg	272.17	J/molxK	628.43	Joback Method
cpg	264.22	J/molxK	594.86	Joback Method
cpg	255.79	J/molxK	561.29	Joback Method
cpg	246.87	J/molxK	527.71	Joback Method
cpg	286.77	J/molxK	695.58	Joback Method
dvisc	0.0003927	Paxs	494.14	Joback Method

dvisc	0.0004929	Paxs	461.29	Joback Method
dvisc	0.0006407	Paxs	428.44	Joback Method
dvisc	0.0008699	Paxs	395.58	Joback Method
dvisc	0.0012484	Paxs	362.73	Joback Method
dvisc	0.0019251	Paxs	329.88	Joback Method
dvisc	0.0032673	Paxs	297.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	2.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22809376&Units=SI

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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