6-BROMOHEXANOYL CHLORIDE

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

Physical Properties

Property code	Value	Unit	Source
hfus	22.38	kJ/mol	Joback Method
ie	9.99	eV	Cheméo Relay (1.0)
logp	2.707		Crippen Method
mcvol	126.710	ml/mol	McGowan Method
tb	497.08	K	Cheméo Relay (1.0)
tf	269.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.45	J/mol×K	494.14	Joback Method
cpg	246.87	J/mol×K	527.71	Joback Method
cpg	255.79	J/mol×K	561.29	Joback Method
cpg	264.22	J/mol×K	594.86	Joback Method
cpg	272.17	J/mol×K	628.43	Joback Method
cpg	279.68	J/mol×K	662.01	Joback Method
cpg	286.77	J/mol×K	695.58	Joback Method
dvisc	0.0032673	Pa×s	297.03	Joback Method
dvisc	0.0019251	Pa×s	329.88	Joback Method
dvisc	0.0012484	Pa×s	362.73	Joback Method
dvisc	0.0008699	Pa×s	395.58	Joback Method
dvisc	0.0006407	Pa×s	428.44	Joback Method
dvisc	0.0004929	Pa×s	461.29	Joback Method
dvisc	0.0003927	Pa×s	494.14	Joback Method

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point