Hexanedioic acid monochloride monomethyl ester

Other names: Methyl adipyl chloride
Methyl 5-(chloroformyl)pentanoate
Hexanoic acid, 6-chloro-6-oxo-, methyl ester
methyl 6-chloro-6-oxohexanoate

Inchi: InChI=1S/C7H11ClO3/c1-11-7(10)5-3-2-4-6(8)9/h2-5H2,1H3

InchiKey: HDLGIEZOMYJKAK-UHFFFAOYSA-N

Formula: C7H11ClO3

SMILES: COC(=O)CCCCC(=O)Cl

Mol. weight [g/mol]: 178.61

CAS: 35444-44-1

Physical Properties

Property code	Value	Unit	Source
gf	-366.71	kJ/mol	Joback Method
hf	-560.93	kJ/mol	Joback Method
hfus	22.47	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.485		Crippen Method
mcvol	130.740	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
tb	527.15	K	Joback Method
tc	719.17	K	Joback Method
tf	320.66	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.52	J/mol×K	527.15	Joback Method
cpg	290.60	J/mol×K	559.15	Joback Method
cpg	300.24	J/mol×K	591.16	Joback Method
cpg	309.43	J/mol×K	623.16	Joback Method
cpg	318.20	J/mol×K	655.16	Joback Method

cpg	326.52	J/mol×K	687.17	Joback Method
cpg	334.41	J/mol×K	719.17	Joback Method
dvisc	0.0025861	Pa×s	320.66	Joback Method
dvisc	0.0015213	Pa×s	355.08	Joback Method
dvisc	0.0009829	Pa×s	389.49	Joback Method
dvisc	0.0006817	Pa×s	423.90	Joback Method
dvisc	0.0004996	Pa×s	458.32	Joback Method
dvisc	0.0003823	Pa×s	492.74	Joback Method
dvisc	0.0003030	Pa×s	527.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35444441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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