

Heptanoic acid, 7-chloro-

Inchi:	InChI=1S/C7H13ClO2/c8-6-4-2-1-3-5-7(9)10/h1-6H2,(H,9,10)
InchiKey:	IGNBKLCFKTYIRI-UHFFFAOYSA-N
Formula:	C7H13ClO2
SMILES:	O=C(O)CCCCCCI
Mol. weight [g/mol]:	164.63
CAS:	821-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-269.61	kJ/mol	Joback Method
hf	-468.36	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	58.99	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.260		Crippen Method
mvol	129.170	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1374.00		NIST Webbook
tb	543.04	K	Joback Method
tc	718.27	K	Joback Method
tf	309.32	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.57	J/molxK	543.04	Joback Method
cpg	300.03	J/molxK	572.24	Joback Method
cpg	309.07	J/molxK	601.45	Joback Method
cpg	317.70	J/molxK	630.65	Joback Method
cpg	325.93	J/molxK	659.86	Joback Method
cpg	333.77	J/molxK	689.06	Joback Method
cpg	341.23	J/molxK	718.27	Joback Method
dvisc	0.0114499	Paxs	309.32	Joback Method

dvisc	0.0037234	Paxs	348.27	Joback Method
dvisc	0.0015179	Paxs	387.23	Joback Method
dvisc	0.0007291	Paxs	426.18	Joback Method
dvisc	0.0003960	Paxs	465.13	Joback Method
dvisc	0.0002363	Paxs	504.09	Joback Method
dvisc	0.0001519	Paxs	543.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821578&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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