

1-Chloroheptan-2-one

Inchi:	InChI=1S/C7H13ClO/c1-2-3-4-5-7(9)6-8/h2-6H2,1H3
InchiKey:	SNVVZCPNLVAKLC-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	CCCCCC(=O)Cl
Mol. weight [g/mol]:	148.63

Physical Properties

Property code	Value	Unit	Source
gf	-132.79	kJ/mol	Joback Method
hf	-316.13	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.375		Crippen Method
mcpvol	123.300	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	450.86	K	Joback Method
tc	634.19	K	Joback Method
tf	248.50	K	Joback Method
vc	0.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.45	J/mol×K	450.86	Joback Method
cpg	253.46	J/mol×K	481.42	Joback Method
cpg	263.99	J/mol×K	511.97	Joback Method
cpg	274.05	J/mol×K	542.53	Joback Method
cpg	283.67	J/mol×K	573.08	Joback Method
cpg	292.85	J/mol×K	603.64	Joback Method
cpg	301.60	J/mol×K	634.19	Joback Method

dvisc	0.0041001	Paxs	248.50	Joback Method
dvisc	0.0021043	Paxs	282.23	Joback Method
dvisc	0.0012453	Paxs	315.95	Joback Method
dvisc	0.0008154	Paxs	349.68	Joback Method
dvisc	0.0005752	Paxs	383.41	Joback Method
dvisc	0.0004293	Paxs	417.13	Joback Method
dvisc	0.0003348	Paxs	450.86	Joback Method

Sources

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=R632856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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