

Cyclopentanecarbonylchloride

Inchi:	InChI=1S/C6H9ClO/c7-6(8)5-3-1-2-4-5/h5H,1-4H2
InchiKey:	WEPUZBYKXNKSDH-UHFFFAOYSA-N
Formula:	C6H9ClO
SMILES:	O=C(Cl)C1CCCC1
Mol. weight [g/mol]:	132.59

Physical Properties

Property code	Value	Unit	Source
hf	-240.23	kJ/mol	Cheméo Relay (1.0)
hfus	11.03	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-2.23		Cheméo Relay (1.0)
logp	1.942		Crippen Method
mcvol	98.350	ml/mol	McGowan Method
tb	435.20	K	Cheméo Relay (1.0)
tf	201.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.38	J/mol×K	443.26	Joback Method
cpg	197.04	J/mol×K	479.48	Joback Method
cpg	208.95	J/mol×K	515.69	Joback Method
cpg	220.13	J/mol×K	551.91	Joback Method
cpg	230.61	J/mol×K	588.13	Joback Method
cpg	240.41	J/mol×K	624.34	Joback Method
cpg	249.58	J/mol×K	660.56	Joback Method
dvisc	0.0038173	Pa×s	248.13	Joback Method
dvisc	0.0021757	Pa×s	280.65	Joback Method
dvisc	0.0013937	Pa×s	313.17	Joback Method
dvisc	0.0009707	Pa×s	345.69	Joback Method
dvisc	0.0007196	Pa×s	378.22	Joback Method
dvisc	0.0005593	Pa×s	410.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.50 ± 0.50	K	2.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4524930&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
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

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