Cycloheptyl chloride

Other names: Cycloheptane, chloro-
Cycloheptyl chloride
Inchi: InChI=1S/C7H13Cl/c8-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey: KMJSGLZXFNSANB-UHFFFAOYSA-N
Formula: C7H13Cl
SMILES: ClC1CCCCCC1
Mol. weight [g/mol]: 132.63

Physical Properties

Property code	Value	Unit	Source
hf	-166.53	kJ/mol	Cheméo Relay (1.0)
hfus	7.82	kJ/mol	Joback Method
hvap	45.02	kJ/mol	Cheméo Relay (1.0)
ie	10.13	eV	Cheméo Relay (1.0)
log10ws	-3.30		Cheméo Relay (1.0)
logp	2.948		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
rinpol	1069.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	442.56	K	Cheméo Relay (1.0)
tf	243.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.90	J/mol×K	420.81	Joback Method
cpg	290.44	J/mol×K	640.54	Joback Method
cpg	277.76	J/mol×K	603.91	Joback Method
cpg	264.28	J/mol×K	567.29	Joback Method
cpg	249.97	J/mol×K	530.67	Joback Method
cpg	234.82	J/mol×K	494.05	Joback Method
cpg	218.80	J/mol×K	457.43	Joback Method
dvisc	0.0009871	Pa×s	311.62	Joback Method

dvisc	0.0002882	Pa×s	420.81	Joback Method
dvisc	0.0004019	Pa×s	384.41	Joback Method
dvisc	0.0006010	Pa×s	348.02	Joback Method
dvisc	0.0127586	Pa×s	202.43	Joback Method
dvisc	0.0018486	Pa×s	275.22	Joback Method
dvisc	0.0041917	Pa×s	238.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2453465&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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