

2H-Pyran, tetrahydro, 3,5-dichloro, # 2

Inchi: InChI=1S/C5H8Cl2O/c6-4-1-5(7)3-8-2-4/h4-5H,1-3H2
InchiKey: CQFLTXQOHZLTRP-UHFFFAOYSA-N
Formula: C5H8Cl2O
SMILES: ClC1COCC(Cl)C1
Mol. weight [g/mol]: 155.02

Physical Properties

Property code	Value	Unit	Source
gf	-102.02	kJ/mol	Joback Method
hf	-276.03	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.621		Crippen Method
mcvol	100.800	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
tb	430.49	K	Joback Method
tc	653.29	K	Joback Method
tf	235.66	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.00	J/molxK	430.49	Joback Method
cpg	193.57	J/molxK	467.62	Joback Method
cpg	205.47	J/molxK	504.76	Joback Method
cpg	216.69	J/molxK	541.89	Joback Method
cpg	227.26	J/molxK	579.02	Joback Method
cpg	237.19	J/molxK	616.16	Joback Method
cpg	246.49	J/molxK	653.29	Joback Method
dvisc	0.0044123	Paxs	235.66	Joback Method

dvisc	0.0023483	Paxs	268.13	Joback Method
dvisc	0.0014322	Paxs	300.60	Joback Method
dvisc	0.0009619	Paxs	333.08	Joback Method
dvisc	0.0006934	Paxs	365.55	Joback Method
dvisc	0.0005273	Paxs	398.02	Joback Method
dvisc	0.0004178	Paxs	430.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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