

(E)-3-Hexen-1-ol, chloroacetate

Inchi:	InChI=1S/C8H13ClO2/c1-2-3-4-5-6-11-8(10)7-9/h3-4H,2,5-7H2,1H3/b4-3+
InchiKey:	WPCPCOLQASJMNK-ONEGZZNKSA-N
Formula:	C8H13ClO2
SMILES:	CCC=CCCOC(=O)CCl
Mol. weight [g/mol]:	176.64

Physical Properties

Property code	Value	Unit	Source
gf	-149.15	kJ/mol	Joback Method
hf	-351.77	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.125		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1177.00		NIST Webbook
rinpol	1177.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
tb	500.32	K	Joback Method
tc	689.35	K	Joback Method
tf	276.92	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.11	J/molxK	500.32	Joback Method
cpg	342.09	J/molxK	657.85	Joback Method
cpg	332.68	J/molxK	626.34	Joback Method
cpg	322.79	J/molxK	594.84	Joback Method
cpg	312.41	J/molxK	563.33	Joback Method
cpg	301.52	J/molxK	531.83	Joback Method

cpg	351.03	J/molxK	689.35	Joback Method
dvisc	0.0002205	Paxs	500.32	Joback Method
dvisc	0.0002842	Paxs	463.09	Joback Method
dvisc	0.0003829	Paxs	425.85	Joback Method
dvisc	0.0005463	Paxs	388.62	Joback Method
dvisc	0.0008404	Paxs	351.39	Joback Method
dvisc	0.0014317	Paxs	314.15	Joback Method
dvisc	0.0028149	Paxs	276.92	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=R26649&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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