

Ethyl chloroatrarate

Inchi:	InChI=1S/C11H13ClO4/c1-4-16-11(15)7-5(2)8(12)10(14)6(3)9(7)13/h13-14H,4H2,1-3H3
InchiKey:	FOBOHPQHGSWBL-UHFFFAOYSA-N
Formula:	C11H13ClO4
SMILES:	CCOC(=O)c1c(C)c(Cl)c(O)c(C)c1O
Mol. weight [g/mol]:	244.67
CAS:	57074-25-6

Physical Properties

Property code	Value	Unit	Source
gf	-429.83	kJ/mol	Joback Method
hf	-683.41	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.545		Crippen Method
mcvol	173.510	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	1952.70		NIST Webbook
rinpol	1952.70		NIST Webbook
tb	767.66	K	Joback Method
tc	1000.30	K	Joback Method
tf	603.23	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.23	J/molxK	767.66	Joback Method
cpg	471.62	J/molxK	806.43	Joback Method
cpg	481.64	J/molxK	845.21	Joback Method
cpg	491.38	J/molxK	883.98	Joback Method
cpg	500.93	J/molxK	922.75	Joback Method
cpg	510.40	J/molxK	961.52	Joback Method
cpg	519.88	J/molxK	1000.30	Joback Method

dvisc	0.0000101	Paxs	603.23	Joback Method
dvisc	0.0000062	Paxs	630.63	Joback Method
dvisc	0.0000039	Paxs	658.04	Joback Method
dvisc	0.0000026	Paxs	685.45	Joback Method
dvisc	0.0000018	Paxs	712.85	Joback Method
dvisc	0.0000013	Paxs	740.26	Joback Method
dvisc	0.0000009	Paxs	767.66	Joback Method

Sources

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=C57074256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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