Carbonic chloride fluoride

Other names:	CARBONYL CHLORIDE FLUORIDE
	COClF
	Carbonyl chlorofluoride
	Cholan-24-oic acid, 3,7-dihydroxy-, (3a,5«beta»,7a)-
	Cholan-24-oic acid, 3,7-dihydroxy-, (3a,5Â«betaÂ»,7a)-
	Estra-1,3,5(10), 7-tetraen-17-one, 3-hydroxy-
Inchi:	InChI=1S/CClFO/c2-1(3)4
InchiKey:	OXVVNXMNLYYMOL-UHFFFAOYSA-N
Formula:	CClFO
SMILES:	O=C(F)Cl
Mol. weight [g/mol]:	82.46
CAS:	353-49-1

Physical Properties

Property code	Value	Unit	Source
gf	-378.12	kJ/mol	Joback Method
hf	-388.40	kJ/mol	Joback Method
hfus	7.22	kJ/mol	Joback Method
hvap	28.13	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.315		Crippen Method
mcvol	40.530	ml/mol	McGowan Method
pc	5627.81	kPa	Joback Method
rinpol	290.00		NIST Webbook
rinpol	290.00		NIST Webbook
tb	312.85	K	Joback Method
tc	490.39	K	Joback Method
tf	181.47	K	Joback Method
vc	0.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	51.71	J/mol×K	312.85	Joback Method

cpg	53.47	J/mol×K	342.44	Joback Method
cpg	55.16	J/mol×K	372.03	Joback Method
cpg	56.78	J/mol×K	401.62	Joback Method
cpg	58.32	J/mol×K	431.21	Joback Method
cpg	59.79	J/mol×K	460.80	Joback Method
cpg	61.19	J/mol×K	490.39	Joback Method
hvapt	22.70	kJ/mol	188.00	NIST Webbook
hvapt	22.00	kJ/mol	192.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.66472e+01
Coeff. B	-2.73363e+03
Temperature range (K), min.	165.00
Temperature range (K), max.	241.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
KDB: https://www.cheric.org/files/research/kdb/mol/mol1768.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C353491&Units=SI

Legend

cpg: Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume