Methoxyflurane

Other names:	2,2-Dichloro-1,1-difluoro-1-methoxyethane
	2,2-Dichloro-1,1-difluoroethyl methyl ether
	Analgizer
	Anecotan
	DA-759
	Ethane, 2,2-dichloro-1,1-difluoro-1-methoxy-
	Ether, 2,2-dichloro-1,1-difluoroethyl methyl
	Ingalan
	Inhalan
	Methofane
	Methoflurane
	Methoxane
	Methoxiflurane
	Methoxyfluran
	Methyl 1,1-difluoro-2,2-dichloroethyl ether
	Metofane
	Metoxfluran
	Metoxifluran
	NSC-110432
	Penthrane
	Pentran
	Pentrane
Inchi:	InChI=1S/C3H4Cl2F2O/c1-8-3(6,7)2(4)5/h2H,1H3
InchiKey:	RFKMCNOHBTXSMU-UHFFFAOYSA-N
Formula:	C3H4Cl2F2O
SMILES:	COC(F)(F)C(Cl)Cl
Mol. weight [g/mol]:	164.97
CAS:	76-38-0

Physical Properties

Property code	Value	Unit	Source
gf	-543.70	kJ/mol	Joback Method
hf	-675.20	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	30.13	kJ/mol	Joback Method
ie	11.50	eV	NIST Webbook

ie	11.00	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	2.029		Crippen Method
mcvol	87.020	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	706.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	722.00		NIST Webbook
rinpol	701.00		NIST Webbook
rinpol	708.00		NIST Webbook
ripol	1124.00		NIST Webbook
tb	360.19	K	Joback Method
tc	538.92	K	Joback Method
tf	194.24	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.92	J/mol×K	360.19	Joback Method
cpg	153.37	J/mol×K	389.98	Joback Method
cpg	159.47	J/mol×K	419.77	Joback Method
cpg	165.23	J/mol×K	449.56	Joback Method
cpg	170.68	J/mol×K	479.35	Joback Method
cpg	175.81	J/mol×K	509.14	Joback Method
cpg	180.64	J/mol×K	538.92	Joback Method
hvapt	40.30	kJ/mol	328.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42817e+01
Coeff. B	-3.07759e+03
Coeff. C	-5.96700e+01
Temperature range (K), min.	279.00

Temperature range (K), max.	402.76

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=C76380&Units=SI
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

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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume