Enflurane

Other names:	Ethane, 2-chloro-1-(difluoromethoxy)-1,1,2-trifluoro- Ether, 2-chloro-1,1,2-trifluoroethyl difluoromethyl Compound 347 Ethrane Ohio 347 2-Chloro-1,1,2-trifluoroethyl difluoromethyl ether 347 Anesthetic Compound No. 347 Anesthetic 347 C 347 Efrane Methylflurether 2-Chloro-1-(difluoromethoxy)-1,1,2-trifluoroethane NSC-115944 2-Chloro-1,1,2-difluoroethane, 1-difluoromethoxy- Alyrane
Inchi:	InChI=1S/C3H2ClF5O/c4-1(5)3(8,9)10-2(6)7/h1-2H
InchiKey:	JPGQOUSTVILISH-UHFFFAOYSA-N
Formula:	C3H2ClF5O
SMILES:	FC(F)OC(F)(F)C(F)Cl
Mol. weight [g/mol]:	184.49
CAS:	13838-16-9

Physical Properties

Property code	Value	Unit	Source
gf	-1118.64	kJ/mol	Joback Method
hf	-1253.07	kJ/mol	Joback Method
hfus	9.85	kJ/mol	Joback Method
hvap	32.74	kJ/mol	NIST Webbook
hvap	32.60 ± 0.10	kJ/mol	NIST Webbook
ie	12.20	eV	NIST Webbook
ie	11.70	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	2.353		Crippen Method
mcvol	80.090	ml/mol	McGowan Method
pc	2980.00 ± 5.00	kPa	NIST Webbook
rinpol	462.00		NIST Webbook

rinpol	494.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	478.00		NIST Webbook
rinpol	486.00		NIST Webbook
rinpol	462.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	840.00		NIST Webbook
tb	330.10	K	NIST Webbook
tb	329.70	K	NIST Webbook
tc	474.30	K	NIST Webbook
tc	475.03 ± 0.02	K	NIST Webbook
tf	151.09	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.82	J/mol×K	465.94	Joback Method
cpg	155.44	J/mol×K	344.43	Joback Method
cpg	161.23	J/mol×K	368.73	Joback Method
cpg	166.76	J/mol×K	393.04	Joback Method
cpg	172.03	J/mol×K	417.34	Joback Method
cpg	177.05	J/mol×K	441.64	Joback Method
cpg	149.38	J/mol×K	320.13	Joback Method
hvapt	30.09	kJ/mol	330.10	NIST Webbook
hvapt	33.80	kJ/mol	312.50	NIST Webbook
hvapt	32.90	kJ/mol	309.50	NIST Webbook
hvapt	31.30 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	30.20 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	29.10 ± 0.10	kJ/mol	343.00	NIST Webbook

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=C13838169&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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