Isoflurane

Other names:	Ethane, 2-chloro-2-(difluoromethoxy)-1,1,1-trifluoro- Ether, 1-chloro-2,2,2-trifluoroethyl difluoromethyl Forane 1-Chloro-2,2,2-trifluoroethyl difluoromethyl ether Aerrane 2-Chloro-2-(difluoromethoxy)-1,1,1-trifluoroethane Compd 469 Compound 469 Forene Ethane, 1-chloro-1-(difluoromethoxy)-2,2,2-trifluoro- IsoFlo R-E 235dal
Inchi:	InChI=1S/C3H2ClF5O/c4-1(3(7,8)9)10-2(5)6/h1-2H
InchiKey:	PIWKPBJCKXDKJR-UHFFFAOYSA-N
Formula:	C3H2ClF5O
SMILES:	FC(F)OC(Cl)C(F)(F)F
Mol. weight [g/mol]:	184.49
CAS:	26675-46-7

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	22.91	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.353		Crippen Method
mcvol	80.090	ml/mol	McGowan Method
pc	3046.00 ± 5.00	kPa	NIST Webbook
rinpol	454.00		NIST Webbook
rinpol	454.00		NIST Webbook
rinpol	454.00		NIST Webbook
tb	321.60	K	NIST Webbook
tc	467.80 ± 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	149.38	J/mol×K	320.13	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	181.82	J/mol×K	465.94	Joback Method
hvapt	31.70	kJ/mol	312.00	NIST Webbook
hvapt	31.90	kJ/mol	297.50	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26675467&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
rinpol: Non-polar retention indices

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