Sevoflurane

Other names: 1,1,1,3,3,3-Hexafluoro-2-fluoromethoxypropane
Inchi: InChI=1S/C4H3F7O/c5-1-12-2(3(6,7)8)4(9,10)11/h2H,1H2
InchiKey: DFEYYRMXOJXZRJ-UHFFFAOYSA-N
Formula: C4H3F7O
SMILES: FCOC(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 200.05
CAS: 28523-86-6

Physical Properties

Property code	Value	Unit	Source
gf	-1482.63	kJ/mol	Joback Method
hf	-1653.66	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	18.21	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.423		Crippen Method
mcvol	85.480	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	301.33	K	Joback Method
tc	429.44	K	Joback Method
tf	151.04	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.91	J/mol×K	301.33	Joback Method
cpg	178.79	J/mol×K	322.68	Joback Method
cpg	186.31	J/mol×K	344.03	Joback Method
cpg	193.50	J/mol×K	365.38	Joback Method
cpg	200.35	J/mol×K	386.74	Joback Method
cpg	206.88	J/mol×K	408.09	Joback Method
cpg	213.09	J/mol×K	429.44	Joback Method

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=C28523866&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume