2,2,2-Trifluoroethyl methyl ether

Other names: CF3CH2OCH3
Inchi: InChI=1S/C3H5F3O/c1-7-2-3(4,5)6/h2H2,1H3
InchiKey: OHLVGBXMHDWRRX-UHFFFAOYSA-N
Formula: C3H5F3O
SMILES: COCC(F)(F)F
Mol. weight [g/mol]: 114.07
CAS: 460-43-5

Physical Properties

Property code	Value	Unit	Source
affp	747.60	kJ/mol	NIST Webbook
basg	718.40	kJ/mol	NIST Webbook
gf	-712.21	kJ/mol	Joback Method
hf	-834.55	kJ/mol	Joback Method
hfus	6.54	kJ/mol	Joback Method
hvap	20.94	kJ/mol	Joback Method
ie	10.53	eV	NIST Webbook
log10ws	-0.83		Crippen Method
logp	1.195		Crippen Method
mcvol	64.310	ml/mol	McGowan Method
pc	3513.00 ± 6.00	kPa	NIST Webbook
rhoc	411.78 ± 4.56	kg/m3	NIST Webbook
tb	304.77 ± 0.10	K	NIST Webbook
tc	448.98 ± 0.08	K	NIST Webbook
tf	149.99	K	Joback Method
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	110.81	J/mol×K	285.04	Joback Method
cpg	116.96	J/mol×K	309.23	Joback Method
cpg	122.87	J/mol×K	333.42	Joback Method
cpg	128.57	J/mol×K	357.61	Joback Method

cpg	134.05	J/mol×K	381.81	Joback Method
cpg	139.31	J/mol×K	406.00	Joback Method
cpg	144.36	J/mol×K	430.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59829e+01
Coeff. B	-3.16951e+03
Coeff. C	-2.58760e+01
Temperature range (K), min.	227.82
Temperature range (K), max.	322.89

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=C460435&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp: Proton affinity

basg: Gas basicity

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

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