Ethanal, trifluoro

Inchi: InChI=1S/C2HF3O/c3-2(4,5)1-6/h1H
InchiKey: JVTSHOJDBRTPHD-UHFFFAOYSA-N
Formula: C2HF3O
SMILES: O=CC(F)(F)F
Mol. weight [g/mol]: 98.02

Physical Properties

Property code	Value	Unit	Source
gf	-715.15	kJ/mol	Joback Method
hf	-767.27	kJ/mol	Joback Method
hfus	5.05	kJ/mol	Joback Method
hvap	23.02	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.748		Crippen Method
mcvol	45.920	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
rinpol	327.00		NIST Webbook
rinpol	327.00		NIST Webbook
tb	288.40	K	Joback Method
tc	441.58	K	Joback Method
tf	158.49	K	Joback Method
vc	0.207	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.81	J/mol×K	288.40	Joback Method
cpg	83.31	J/mol×K	313.93	Joback Method
cpg	87.55	J/mol×K	339.46	Joback Method
cpg	91.53	J/mol×K	364.99	Joback Method
cpg	95.26	J/mol×K	390.52	Joback Method
cpg	98.75	J/mol×K	416.05	Joback Method
cpg	102.01	J/mol×K	441.58	Joback Method

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=R511610&Units=SI
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
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