ETHYL FLUOROFORMATE

Other names: FCO2C2H5
Inchi: InChI=1S/C3H5FO2/c1-2-6-3(4)5/h2H2,1H3
InchiKey: PWEHMQBAMSTRDF-UHFFFAOYSA-N
Formula: C3H5FO2
SMILES: CCOC(=O)F
Mol. weight [g/mol]: 92.07

Physical Properties

Property code	Value	Unit	Source
af	0.3437		Cheméo Relay (1.0)
affp	757.00	kJ/mol	NIST Webbook
basg	726.00	kJ/mol	NIST Webbook
gf	-454.35	kJ/mol	Joback Method
hf	-636.61	kJ/mol	Cheméo Relay (1.0)
hfus	9.39	kJ/mol	Joback Method
hvap	28.42	kJ/mol	Cheméo Relay (1.0)
ie	11.25	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.112		Crippen Method
mcvol	62.340	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	329.50 ± 3.00	K	NIST Webbook
tc	452.25	K	Cheméo Relay (1.0)
tf	162.59	K	Cheméo Relay (1.0)
vc	0.233	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.62	J/mol×K	343.60	Joback Method
cpg	111.64	J/mol×K	371.85	Joback Method
cpg	116.56	J/mol×K	400.10	Joback Method
cpg	121.38	J/mol×K	428.35	Joback Method
cpg	126.08	J/mol×K	456.60	Joback Method

cpg	130.67	J/mol×K	484.85	Joback Method
cpg	135.13	J/mol×K	513.10	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461643&Units=SI

Legend

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