Acetic acid, difluoro-, ethyl ester

Other names: Ethyl difluoroacetate
Inchi: InChI=1S/C4H6F2O2/c1-2-8-4(7)3(5)6/h3H,2H2,1H3
InchiKey: GZKHDVAKKLTJPO-UHFFFAOYSA-N
Formula: C4H6F2O2
SMILES: CCOC(=O)C(F)F
Mol. weight [g/mol]: 124.09
CAS: 454-31-9

Physical Properties

Property code	Value	Unit	Source
chl	-1939.10	kJ/mol	NIST Webbook
gf	-643.18	kJ/mol	Joback Method
hf	-768.19	kJ/mol	Joback Method
hfus	11.54	kJ/mol	Joback Method
hvap	31.63	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.815		Crippen Method
mcvol	78.200	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	365.31	K	Joback Method
tc	529.44	K	Joback Method
tf	193.18	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.11	J/mol×K	365.31	Joback Method
cpg	152.65	J/mol×K	392.66	Joback Method
cpg	159.01	J/mol×K	420.02	Joback Method
cpg	165.19	J/mol×K	447.37	Joback Method
cpg	171.18	J/mol×K	474.73	Joback Method
cpg	176.99	J/mol×K	502.08	Joback Method
cpg	182.61	J/mol×K	529.44	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=C454319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
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