

Acetic acid, fluoro-, ethyl ester

Other names:	Ethyl fluoroacetate Ethyl monofluoroacetate Ethylester kyseliny fluoroctove Fluoroacetic acid ethyl ester
Inchi:	InChI=1S/C4H7FO2/c1-2-7-4(6)3-5/h2-3H2,1H3
InchiKey:	VCYZVXRKYPKDQB-UHFFFAOYSA-N
Formula:	C4H7FO2
SMILES:	CCOC(=O)CF
Mol. weight [g/mol]:	106.10
CAS:	459-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-445.93	kJ/mol	Joback Method
hf	-566.80	kJ/mol	Joback Method
hfus	11.98	kJ/mol	Joback Method
hvap	32.84	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.519		Crippen Method
mcvol	76.430	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	366.48	K	Joback Method
tc	535.95	K	Joback Method
tf	207.59	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.88	J/molxK	366.48	Joback Method
cpg	144.48	J/molxK	394.72	Joback Method
cpg	150.91	J/molxK	422.97	Joback Method
cpg	157.16	J/molxK	451.21	Joback Method
cpg	163.25	J/molxK	479.46	Joback Method

cpg	169.15	J/mol×K	507.70	Joback Method
cpg	174.87	J/mol×K	535.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.74382e+01
Coeff. B	-5.04013e+03
Temperature range (K), min.	273.00
Temperature range (K), max.	415.62

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C459723&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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