Acetic acid, difluoro-, methyl ester

Other names: methyl difluoroacetate
Inchi: InChI=1S/C3H4F2O2/c1-7-3(6)2(4)5/h2H,1H3
InchiKey: CSSYKHYGURSRAZ-UHFFFAOYSA-N
Formula: C3H4F2O2
SMILES: COC(=O)C(F)F
Mol. weight [g/mol]: 110.06
CAS: 433-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-651.60	kJ/mol	Joback Method
hf	-747.55	kJ/mol	Joback Method
hfus	8.95	kJ/mol	Joback Method
hvap	29.41	kJ/mol	Joback Method
log10ws	-0.25		Crippen Method
logp	0.424		Crippen Method
mcvol	64.110	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
tb	358.50 ± 0.50	K	NIST Webbook
tc	506.42	K	Joback Method
tf	181.91	K	Joback Method
vc	0.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.69	J/mol×K	479.09	Joback Method
cpg	114.78	J/mol×K	342.43	Joback Method
cpg	119.80	J/mol×K	369.76	Joback Method
cpg	124.71	J/mol×K	397.09	Joback Method
cpg	129.49	J/mol×K	424.42	Joback Method
cpg	134.16	J/mol×K	451.75	Joback Method
cpg	143.10	J/mol×K	506.42	Joback Method
hvapt	41.90	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.86708e+01
Coeff. B	-5.03783e+03
Temperature range (K), min.	273.00
Temperature range (K), max.	377.10

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=C433534&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
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