

FLUOROACETIC ACID, METHYL ESTER

Other names:	Acetic acid, fluoro-, methyl ester Fluoracetic acid methyl ester MFA Methyl fluoroacetate Methylester kyseliny fluoroctove TL 551
Inchi:	InChI=1S/C3H5FO2/c1-6-3(5)2-4/h2H2,1H3
InchiKey:	RJBYSQHLLIHSLT-UHFFFAOYSA-N
Formula:	C3H5FO2
SMILES:	COC(=O)CF
Mol. weight [g/mol]:	92.07
CAS:	453-18-9

Physical Properties

Property code	Value	Unit	Source
af	0.3585		Cheméo Relay (1.0)
hf	-591.47	kJ/mol	Cheméo Relay (1.0)
hfus	9.39	kJ/mol	Joback Method
hvap	31.28	kJ/mol	Cheméo Relay (1.0)
ie	10.40	eV	Cheméo Relay (1.0)
log10ws	0.36		Cheméo Relay (1.0)
logp	0.129		Crippen Method
mcvol	62.340	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	377.70	K	NIST Webbook
tc	523.74	K	Cheméo Relay (1.0)
tf	207.88	K	Cheméo Relay (1.0)
vc	0.231	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
hvapt	42.70	kJ/mol	303.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.81981e+01
Coeff. B	-5.12838e+03
Temperature range (K), min.	273.00
Temperature range (K), max.	397.96

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C453189&Units=SI>

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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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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