Methyl trifluoroacetate

Other names: Trifluoroacetic acid methyl ester
Acetic acid, trifluoro-, methyl ester
CF3C(O)OCH3
Inchi: InChI=1S/C3H3F3O2/c1-8-2(7)3(4,5)6/h1H3
InchiKey: VMVNZNXAVJHNDJ-UHFFFAOYSA-N
Formula: C3H3F3O2
SMILES: COC(=O)C(F)(F)F
Mol. weight [g/mol]: 128.05
CAS: 431-47-0

Physical Properties

Property code	Value	Unit	Source
affp	740.50	kJ/mol	NIST Webbook
basg	709.60	kJ/mol	NIST Webbook
gf	-841.13	kJ/mol	Joback Method
hf	-992.90 ± 5.40	kJ/mol	NIST Webbook
hfl	-1020.00 ± 5.90	kJ/mol	NIST Webbook
hfus	8.14	kJ/mol	Joback Method
hvap	28.00 ± 3.00	kJ/mol	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.722		Crippen Method
mcvol	65.880	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	400.00		NIST Webbook
rinpol	400.40		NIST Webbook
rinpol	400.00		NIST Webbook
tb	316.50	K	NIST Webbook
tb	316.50 ± 0.50	K	NIST Webbook
tc	500.44	K	Joback Method
tf	199.92	K	Joback Method
vc	0.271	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.85	J/mol×K	338.91	Joback Method
cpg	129.63	J/mol×K	365.83	Joback Method
cpg	135.15	J/mol×K	392.75	Joback Method
cpg	140.42	J/mol×K	419.67	Joback Method
cpg	145.45	J/mol×K	446.59	Joback Method
cpg	150.24	J/mol×K	473.52	Joback Method
cpg	154.80	J/mol×K	500.44	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=C431470&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
hfl: Liquid phase 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume