Methyl 4,4,4-trifluorocrotonate

Inchi: InChI=1S/C5H5F3O2/c1-10-4(9)2-3-5(6,7)8/h2-3H,1H3/b3-2+
InchiKey: DMMZYYLXAGRBDO-NSCUHMNNSA-N
Formula: C5H5F3O2
SMILES: COC(=O)C=CC(F)(F)F
Mol. weight [g/mol]: 154.09
CAS: 85694-31-1

Physical Properties

Property code	Value	Unit	Source
gf	-744.07	kJ/mol	Joback Method
hf	-871.19	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	32.09	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.278		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	388.83	K	Joback Method
tc	558.79	K	Joback Method
tf	217.38	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.08	J/mol×K	388.83	Joback Method
cpg	183.20	J/mol×K	417.16	Joback Method
cpg	190.87	J/mol×K	445.48	Joback Method
cpg	198.13	J/mol×K	473.81	Joback Method
cpg	204.98	J/mol×K	502.14	Joback Method
cpg	211.44	J/mol×K	530.46	Joback Method
cpg	217.53	J/mol×K	558.79	Joback Method

Sources

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=C85694311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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