

acetyl fluoride

Inchi: InChI=1S/C2H3FO/c1-2(3)4/h1H3
InchiKey: JUCMRTZQCZRJDC-UHFFFAOYSA-N
Formula: C2H3FO
SMILES: CC(=O)F
Mol. weight [g/mol]: 62.04
CAS: 557-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-357.77	kJ/mol	Joback Method
hf	-445.00 ± 2.00	kJ/mol	NIST Webbook
hf	-437.60	kJ/mol	NIST Webbook
hfl	-470.30 ± 0.40	kJ/mol	NIST Webbook
hfl	-463.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-466.39 ± 0.08	kJ/mol	NIST Webbook
hfus	5.62	kJ/mol	Joback Method
hvap	30.00	kJ/mol	NIST Webbook
hvap	25.00 ± 2.00	kJ/mol	NIST Webbook
ie	11.51 ± 0.02	eV	NIST Webbook
log10ws	-0.29		Crippen Method
logp	0.502		Crippen Method
mcvol	42.380	ml/mol	McGowan Method
pc	5160.85	kPa	Joback Method
tb	294.00	K	NIST Webbook
tb	295.00 ± 2.00	K	NIST Webbook
tb	293.00	K	NIST Webbook
tb	293.50 ± 0.50	K	NIST Webbook
tc	465.37	K	Joback Method
tf	162.82	K	Joback Method
vc	0.172	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	60.39	J/mol×K	298.30	Joback Method
cpg	63.97	J/mol×K	326.15	Joback Method
cpg	67.44	J/mol×K	353.99	Joback Method
cpg	70.79	J/mol×K	381.84	Joback Method
cpg	74.04	J/mol×K	409.68	Joback Method
cpg	77.17	J/mol×K	437.53	Joback Method
cpg	80.19	J/mol×K	465.37	Joback Method
hvapt	14.30	kJ/mol	238.00	NIST Webbook

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=C557993&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
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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