

CF₂HCON(CH₃)₂

Inchi: InChI=1S/C4H7F2NO/c1-7(2)4(8)3(5)6/h3H,1-2H3
InchiKey: IUEWOPMXNADAEB-UHFFFAOYSA-N
Formula: C₄H₇F₂NO
SMILES: CN(C)C(=O)C(F)F
Mol. weight [g/mol]: 123.10
CAS: 667-50-5

Physical Properties

Property code	Value	Unit	Source
affp	864.10	kJ/mol	NIST Webbook
basg	833.10	kJ/mol	NIST Webbook
gf	-427.40	kJ/mol	Joback Method
hf	-568.44	kJ/mol	Joback Method
hfus	13.37	kJ/mol	Joback Method
hvap	31.27	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	0.340		Crippen Method
mcvol	82.310	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	355.33	K	Joback Method
tc	517.50	K	Joback Method
tf	203.42	K	Joback Method
vc	0.314	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.88	J/mol×K	355.33	Joback Method
cpg	158.03	J/mol×K	382.36	Joback Method
cpg	165.82	J/mol×K	409.39	Joback Method
cpg	173.28	J/mol×K	436.41	Joback Method
cpg	180.41	J/mol×K	463.44	Joback Method
cpg	187.22	J/mol×K	490.47	Joback Method
cpg	193.72	J/mol×K	517.50	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=C667505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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