

Methylene, difluoro-

Other names:	Calcium difluoride Difluoromethylene
Inchi:	InChI=1S/CF2/c2-1-3
InchiKey:	LTVOKYUPTHZZQH-UHFFFAOYSA-N
Formula:	CF2
SMILES:	F[C]F
Mol. weight [g/mol]:	50.01
CAS:	2154-59-8

Physical Properties

Property code	Value	Unit	Source
affp	765.00	kJ/mol	NIST Webbook
basg	732.50	kJ/mol	NIST Webbook
ea	2.65	eV	NIST Webbook
ea	0.20	eV	NIST Webbook
ea	1.30 ± 0.80	eV	NIST Webbook
ea	0.07 ± 0.15	eV	NIST Webbook
ea	0.18 ± 0.01	eV	NIST Webbook
ea	0.18 ± 0.02	eV	NIST Webbook
hf	-172.00 ± 8.40	kJ/mol	NIST Webbook
ie	11.54 ± 0.10	eV	NIST Webbook
ie	11.70 ± 0.20	eV	NIST Webbook
ie	11.80 ± 0.30	eV	NIST Webbook
ie	9.74	eV	NIST Webbook
ie	11.70 ± 0.10	eV	NIST Webbook
ie	11.44 ± 0.03	eV	NIST Webbook
ie	11.45 ± 0.03	eV	NIST Webbook
ie	15.20	eV	NIST Webbook
ie	11.42 ± 0.01	eV	NIST Webbook
ie	11.50 ± 0.10	eV	NIST Webbook
ie	11.40 ± 0.30	eV	NIST Webbook
ie	11.50 ± 0.40	eV	NIST Webbook
ie	11.90 ± 0.10	eV	NIST Webbook
log10ws	-0.50		Crippen Method
logp	0.922		Crippen Method
mcvol	24.190	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2154598&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
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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