Difluoromethyl radical

Inchi: InChI=1S/CHF2/c2-1-3/h1H
InchiKey: JNCMHMUGTWEVOZ-UHFFFAOYSA-N
Formula: CHF2
SMILES: F[CH]F
Mol. weight [g/mol]: 51.02
CAS: 2670-13-5

Physical Properties

Property code	Value	Unit	Source
ea	1.21 ± 0.16	eV	NIST Webbook
gf	-382.14	kJ/mol	Joback Method
hf	-405.66	kJ/mol	Joback Method
hfus	2.67	kJ/mol	Joback Method
hvap	15.65	kJ/mol	Joback Method
ie	8.74	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.45	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
log10ws	-0.55		Crippen Method
logp	1.045		Crippen Method
mcvol	26.340	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
tb	219.68	K	Joback Method
tc	354.46	K	Joback Method
tf	103.58	K	Joback Method
vc	0.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	30.95	J/mol×K	219.68	Joback Method
cpg	33.74	J/mol×K	242.14	Joback Method

cpg	36.34	J/mol×K	264.61	Joback Method
cpg	38.76	J/mol×K	287.07	Joback Method
cpg	41.00	J/mol×K	309.53	Joback Method
cpg	43.08	J/mol×K	332.00	Joback Method
cpg	45.01	J/mol×K	354.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2670135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
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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