Difluoroacetic acid

Other names: Acetic acid, difluoro-
Inchi: InChI=1S/C2H2F2O2/c3-1(4)2(5)6/h1H,(H,5,6)
InchiKey: PBWZKZYHONABLN-UHFFFAOYSA-N
Formula: C2H2F2O2
SMILES: O=C(O)C(F)F
Mol. weight [g/mol]: 96.03
CAS: 381-73-7

Physical Properties

Property code	Value	Unit	Source
chl	-562.96	kJ/mol	NIST Webbook
gf	-691.84	kJ/mol	Joback Method
hf	-746.92	kJ/mol	Joback Method
hfus	9.26	kJ/mol	Joback Method
hvap	41.45	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	0.336		Crippen Method
mcvol	50.020	ml/mol	McGowan Method
pc	5594.19	kPa	Joback Method
tb	406.20	K	NIST Webbook
tb	407.00	K	NIST Webbook
tb	407.00	K	NIST Webbook
tc	550.87	K	Joback Method
tf	209.23	K	Joback Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.80	J/mol×K	389.31	Joback Method
cpg	98.41	J/mol×K	416.24	Joback Method
cpg	101.87	J/mol×K	443.16	Joback Method
cpg	105.19	J/mol×K	470.09	Joback Method
cpg	108.36	J/mol×K	497.02	Joback Method

cpg	111.39	J/mol×K	523.95	Joback Method
cpg	114.29	J/mol×K	550.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.70	K	2.70	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C381737&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume