2,2-Difluoroethanol

Other names: Difluoroethanol
ethanol, 2,2-difluoro-
Inchi: InChI=1S/C2H4F2O/c3-2(4)1-5/h2,5H,1H2
InchiKey: VOGSDFLJZPNWHY-UHFFFAOYSA-N
Formula: C2H4F2O
SMILES: OCC(F)F
Mol. weight [g/mol]: 82.05

Physical Properties

Property code	Value	Unit	Source
affp	727.40	kJ/mol	NIST Webbook
basg	697.00	kJ/mol	NIST Webbook
chl	-1028.20	kJ/mol	NIST Webbook
hf	-653.05	kJ/mol	Cheméo Relay (1.0)
hfus	7.66	kJ/mol	Joback Method
logp	0.244		Crippen Method
mcvol	48.450	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
rinpol	481.00		NIST Webbook
tb	368.50 ± 0.50	K	NIST Webbook
tb	368.50 ± 0.50	K	NIST Webbook
tb	368.70	K	NIST Webbook
tc	549.66	K	Cheméo Relay (1.0)
tf	242.46	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	87.38	J/mol×K	335.44	Joback Method
cpg	91.43	J/mol×K	360.13	Joback Method
cpg	95.34	J/mol×K	384.82	Joback Method
cpg	99.11	J/mol×K	409.50	Joback Method
cpg	102.75	J/mol×K	434.19	Joback Method
cpg	106.25	J/mol×K	458.88	Joback Method

cpg	109.62	J/mol×K	483.57	Joback Method

Sources

Henry s Law Constants of Organic Compounds in Water and n-Octane at T = 293.2 K:	https://www.doi.org/10.1021/je900711h
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C359137&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point