

2,6-DIFLUOROPHENYLACETIC ACID

Other names:	Benzeneacetic acid, 2,6-difluoro-
Inchi:	InChI=1S/C8H6F2O2/c9-6-2-1-3-7(10)5(6)4-8(11)12/h1-3H,4H2,(H,11,12)
InchiKey:	FUGDCKXBUZFEON-UHFFFAOYSA-N
Formula:	C8H6F2O2
SMILES:	O=C(O)Cc1c(F)cccc1F
Mol. weight [g/mol]:	172.13

Physical Properties

Property code	Value	Unit	Source
hfus	21.59	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.592		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
tb	518.32	K	Cheméo Relay (1.0)
tf	396.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.48	J/mol×K	563.67	Joback Method
cpg	259.65	J/mol×K	595.28	Joback Method
cpg	267.37	J/mol×K	626.88	Joback Method
cpg	274.66	J/mol×K	658.49	Joback Method
cpg	281.52	J/mol×K	690.09	Joback Method
cpg	287.98	J/mol×K	721.70	Joback Method
cpg	294.04	J/mol×K	753.30	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85068286&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/63-001-0/2-6-DIFLUOROPHENYLACETIC-ACID.pdf>

Generated by Cheméo on 2026-07-21 20:51:55.999569414 +0000 UTC m=+178211.841454789.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.