

Benzeneacetic acid, 4-fluoro-

Other names:	Acetic acid, (p-fluorophenyl)- (p-Fluorophenyl)acetic acid (4-Fluorophenyl)acetic acid Ba 2821 4-Fluorobenzeneacetic acid
Inchi:	InChI=1S/C8H7FO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey:	MGKPFALCNDRSQD-UHFFFAOYSA-N
Formula:	C8H7FO2
SMILES:	O=C(O)Cc1ccc(F)cc1
Mol. weight [g/mol]:	154.14
CAS:	405-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-341.29	kJ/mol	Joback Method
hf	-444.31	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.453		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
tb	559.42	K	Joback Method
tc	757.03	K	Joback Method
tf	367.00 ± 3.00	K	NIST Webbook
vc	0.418	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.17	J/mol×K	559.42	Joback Method
cpg	253.02	J/mol×K	592.36	Joback Method
cpg	261.35	J/mol×K	625.29	Joback Method
cpg	269.17	J/mol×K	658.23	Joback Method

cpg	276.51	J/mol×K	691.16	Joback Method
cpg	283.38	J/mol×K	724.10	Joback Method
cpg	289.80	J/mol×K	757.03	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	0.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C405505&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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