

Benzeneacetonitrile, 4-fluoro-

Other names:	Acetonitrile, (p-fluorophenyl)- (p-Fluorophenyl)acetonitrile p-Fluorobenzyl cyanide 4-Fluorobenzeneacetonitrile para-Fluorophenylacetonitrile 4-Fluorophenylacetonitrile 4-Fluorobenzyl cyanide 4-Fluorophenylacetic acid nitrile
Inchi:	InChI=1S/C8H6FN/c9-8-3-1-7(2-4-8)5-6-10/h1-4H,5H2
InchiKey:	JHQBLYITVCBGTO-UHFFFAOYSA-N
Formula:	C8H6FN
SMILES:	<chem>N#CCc1ccc(F)cc1</chem>
Mol. weight [g/mol]:	135.14
CAS:	459-22-3

Physical Properties

Property code	Value	Unit	Source
gf	57.63	kJ/mol	Joback Method
hf	-14.62	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	46.00	kJ/mol	Joback Method
ie	9.65 ± 0.04	eV	NIST Webbook
log10ws	-2.47		Crippen Method
logp	1.892		Crippen Method
mcvol	102.970	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	515.45	K	Joback Method
tc	736.16	K	Joback Method
tf	284.44	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	209.53	J/mol×K	515.45	Joback Method
cpg	219.03	J/mol×K	552.24	Joback Method
cpg	227.93	J/mol×K	589.02	Joback Method
cpg	236.26	J/mol×K	625.81	Joback Method
cpg	244.04	J/mol×K	662.59	Joback Method
cpg	251.29	J/mol×K	699.38	Joback Method
cpg	258.04	J/mol×K	736.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.70	K	2.40	NIST Webbook

Sources

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=C459223&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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