Benzeneacetonitrile, 5-fluoro-2-nitro-

Other names: Acetonitrile, (5-fluoro-2-nitrophenyl)-
5-Fluoro-2-nitrophenylacetonitrile
Acetonitrile, 2-(5-fluoro-2-nitrophenyl)-
Inchi: InChI=1S/C8H5FN2O2/c9-7-1-2-8(11(12)13)6(5-7)3-4-10/h1-2,5H,3H2
InchiKey: YETOJTGGLXHUCS-UHFFFAOYSA-N
Formula: C8H5FN2O2
SMILES: N#CCc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]: 180.14
CAS: 3456-75-5

Physical Properties

Property code	Value	Unit	Source
gf	83.55	kJ/mol	Joback Method
hf	-36.85	kJ/mol	Joback Method
hfus	25.69	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	1.800		Crippen Method
mcvol	120.390	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
tb	672.27	K	Joback Method
tc	918.76	K	Joback Method
tf	440.57	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.90	J/mol×K	672.27	Joback Method
cpg	294.50	J/mol×K	713.35	Joback Method
cpg	302.42	J/mol×K	754.43	Joback Method
cpg	309.68	J/mol×K	795.51	Joback Method
cpg	316.33	J/mol×K	836.59	Joback Method
cpg	322.38	J/mol×K	877.68	Joback Method

cpg	327.87	J/mol×K	918.76	Joback Method

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=C3456755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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