

2,3,4,5,6-Pentafluorophenylacetonitrile

Other names:	Pentafluorophenylacetonitrile Benzeneacetonitrile, 2,3,4,5,6-pentafluoro-
Inchi:	InChI=1S/C8H2F5N/c9-4-3(1-2-14)5(10)7(12)8(13)6(4)11/h1H2
InchiKey:	YDNOJUAQBFXZCR-UHFFFAOYSA-N
Formula:	C8H2F5N
SMILES:	N#CCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	207.10
CAS:	653-30-5

Physical Properties

Property code	Value	Unit	Source
gf	-760.13	kJ/mol	Joback Method
hf	-844.94	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	45.38	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.448		Crippen Method
mvol	110.050	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	532.45	K	Joback Method
tc	717.16	K	Joback Method
tf	336.88	K	Joback Method
vc	0.491	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.74	J/mol×K	532.45	Joback Method
cpg	246.31	J/mol×K	563.24	Joback Method
cpg	252.61	J/mol×K	594.02	Joback Method
cpg	258.63	J/mol×K	624.81	Joback Method
cpg	264.38	J/mol×K	655.59	Joback Method
cpg	269.85	J/mol×K	686.38	Joback Method
cpg	275.05	J/mol×K	717.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.00 ± 2.00	K	2.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C653305&Units=SI

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
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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