2-Fluoro-4-(trifluoromethyl)benzonitrile

Other names: «alpha»,«alpha»,«alpha»,2-Tetrafluoro-p-tolunitrile
Inchi: InChI=1S/C8H3F4N/c9-7-3-6(8(10,11)12)2-1-5(7)4-13/h1-3H
InchiKey: JLTYVTXTSOYXMX-UHFFFAOYSA-N
Formula: C8H3F4N
SMILES: N#Cc1ccc(C(F)(F)F)cc1F
Mol. weight [g/mol]: 189.11
CAS: 146070-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-533.59	kJ/mol	Joback Method
hf	-623.17	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	42.92	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.716		Crippen Method
mcvol	108.280	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	515.01	K	Joback Method
tc	717.26	K	Joback Method
tf	301.15	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.76	J/mol×K	515.01	Joback Method
cpg	246.24	J/mol×K	548.72	Joback Method
cpg	254.09	J/mol×K	582.43	Joback Method
cpg	261.36	J/mol×K	616.14	Joback Method
cpg	268.08	J/mol×K	649.84	Joback Method
cpg	274.29	J/mol×K	683.55	Joback Method
cpg	280.01	J/mol×K	717.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146070340&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

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