.ALPHA.,.alpha.,.alpha.,2-tetrafluoro-m-tolunitrile

Other names: 2-Fluoro-3-(trifluoromethyl)benzonitrile
Inchi: InChI=1S/C8H3F4N/c9-7-5(4-13)2-1-3-6(7)8(10,11)12/h1-3H
InchiKey: NMWOWGXPPBIZNH-UHFFFAOYSA-N
Formula: C8H3F4N
SMILES: N#Cc1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 189.11

Physical Properties

Property code	Value	Unit	Source
hf	-617.42	kJ/mol	Cheméo Relay (1.0)
hfus	16.15	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Cheméo Relay (1.0)
ie	10.29	eV	Cheméo Relay (1.0)
log10ws	-2.78		Cheméo Relay (1.0)
logp	2.716		Crippen Method
mcvol	108.280	ml/mol	McGowan Method
tb	459.24	K	Cheméo Relay (1.0)
tf	287.84	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C146070351&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point