

ALPHA,ALPHA,ALPHA,6-TETRAFLUORO-O-TOLU

Other names:	2-Fluoro-6-(trifluoromethyl)benzonitrile
Inchi:	InChI=1S/C8H3F4N/c9-7-3-1-2-6(5(7)4-13)8(10,11)12/h1-3H
InchiKey:	OGQYJDHTHFAPRN-UHFFFAOYSA-N
Formula:	C8H3F4N
SMILES:	N#Cc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]:	189.11

Physical Properties

Property code	Value	Unit	Source
hfus	16.15	kJ/mol	Joback Method
hvap	52.97	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
logp	2.716		Crippen Method
mcvol	108.280	ml/mol	McGowan Method
tb	459.38	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

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C133116833&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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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