

ALPHA,ALPHA,ALPHA,2-TETRAFLUORO-P-TOLU

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

Physical Properties

Property code	Value	Unit	Source
hfus	16.15	kJ/mol	Joback Method
ie	10.43	eV	Cheméo Relay (1.0)
logp	2.716		Crippen Method
mcvol	108.280	ml/mol	McGowan Method
tb	453.37	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

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):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C146070340&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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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