«alpha»,«alpha»,«alpha»-Trifluoro-o-tolunitrile

Other names:	o-Trifluoromethylbenzonitrile
	2-Trifluoromethylbenzonitrile
	Benzonitrile, 2-(trifluoromethyl)-
	o-Tolunitrile, alpha,alpha,alpha-trifluoro-
	alpha,alpha,alpha-Trifluoro-o-tolunitrile
	«alpha»,«alpha»,«alpha»-trifluoro-2-toluonitrile
Inchi:	InChI=1S/C8H4F3N/c9-8(10,11)7-4-2-1-3-6(7)5-12/h1-4H
InchiKey:	SOZGHDCEWOLLHV-UHFFFAOYSA-N
Formula:	C8H4F3N
SMILES:	N#Cc1ccccc1C(F)(F)F
Mol. weight [g/mol]:	171.12
CAS:	447-60-9

Physical Properties

Property code	Value	Unit	Source
ea	0.70 ± 0.10	eV	NIST Webbook
gf	-329.15	kJ/mol	Joback Method
hf	-415.59	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	43.07	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.577		Crippen Method
mcvol	106.510	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
tb	478.00 ± 1.00	K	NIST Webbook
tc	722.52	K	Joback Method
tf	288.04	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.98	J/mol×K	510.76	Joback Method
cpg	239.29	J/mol×K	546.05	Joback Method

cpg	247.87	J/mol×K	581.35	Joback Method
cpg	255.76	J/mol×K	616.64	Joback Method
cpg	263.01	J/mol×K	651.93	Joback Method
cpg	269.67	J/mol×K	687.23	Joback Method
cpg	275.78	J/mol×K	722.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C447609&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
ea:	Electron affinity
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