4-(Trifluoromethoxy)phenylacetonitrile

Other names: p-Trifluoromethoxyphenyl acetonitrile
Inchi: InChI=1S/C9H6F3NO/c10-9(11,12)14-8-3-1-7(2-4-8)5-6-13/h1-4H,5H2
InchiKey: LYFCAROXYJTUQF-UHFFFAOYSA-N
Formula: C9H6F3NO
SMILES: N#CCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 201.15
CAS: 49561-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-425.73	kJ/mol	Joback Method
hf	-568.45	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	47.71	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.651		Crippen Method
mcvol	126.470	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	556.06	K	Joback Method
tc	762.45	K	Joback Method
tf	321.54	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.19	J/mol×K	556.06	Joback Method
cpg	304.24	J/mol×K	590.46	Joback Method
cpg	313.60	J/mol×K	624.86	Joback Method
cpg	322.31	J/mol×K	659.25	Joback Method
cpg	330.39	J/mol×K	693.65	Joback Method
cpg	337.88	J/mol×K	728.05	Joback Method
cpg	344.81	J/mol×K	762.45	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C49561968&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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