

3-(Trifluoromethyl)phenoxyacetonitrile

Inchi:	InChI=1S/C9H6F3NO/c10-9(11,12)7-2-1-3-8(6-7)14-5-4-13/h1-3,6H,5H2
InchiKey:	UGZFDPFADQHEMW-UHFFFAOYSA-N
Formula:	C9H6F3NO
SMILES:	N#CCOc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	201.15

Physical Properties

Property code	Value	Unit	Source
hf	-586.91	kJ/mol	Cheméo Relay (1.0)
hfus	17.24	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Cheméo Relay (1.0)
ie	9.43	eV	Cheméo Relay (1.0)
log10ws	-2.83		Cheméo Relay (1.0)
logp	2.608		Crippen Method
mcvol	126.470	ml/mol	McGowan Method
tb	486.83	K	Cheméo Relay (1.0)
tf	321.31	K	Cheméo Relay (1.0)

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

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=C2145315&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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