

4-(TRIFLUOROMETHYL)PHENYLACETONITRILE

Other names:	p-Trifluoromethylphenylacetonitrile Benzeneacetonitrile, 4-(trifluoromethyl)-
Inchi:	InChI=1S/C9H6F3N/c10-9(11,12)8-3-1-7(2-4-8)5-6-13/h1-4H,5H2
InchiKey:	QNKOCFJZJWOXDE-UHFFFAOYSA-N
Formula:	C9H6F3N
SMILES:	N#CCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	185.15

Physical Properties

Property code	Value	Unit	Source
hfus	16.05	kJ/mol	Joback Method
hvap	61.97	kJ/mol	Cheméo Relay (1.0)
ie	9.87	eV	Cheméo Relay (1.0)
logp	2.771		Crippen Method
mcvol	120.600	ml/mol	McGowan Method
tb	490.09	K	Cheméo Relay (1.0)
tf	327.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.20	J/mol×K	533.64	Joback Method
cpg	282.50	J/mol×K	568.38	Joback Method
cpg	292.03	J/mol×K	603.13	Joback Method
cpg	300.84	J/mol×K	637.87	Joback Method
cpg	308.99	J/mol×K	672.62	Joback Method
cpg	316.51	J/mol×K	707.36	Joback Method
cpg	323.45	J/mol×K	742.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.00 ± 1.00	K	1.60	NIST Webbook

Sources

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=C2338752&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

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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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