Benzeneacetonitrile, 3-(trifluoromethyl)-

Other names:	Acetonitrile, («alpha»,«alpha»,«alpha»-trifluoro-m-tolyl)- («alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl)acetonitrile m-(Trifluoromethyl)benzylcyanide m-Trifluoromethylphenylacetonitrile [3-(Trifluoromethyl)phenyl]acetonitrile 3-(Trifluoromethyl)benzeneacetonitrile 3-(Trifluoromethyl)benzyl cyanide 3-Trifluormethylbenzylcyanide
Inchi:	InChI=1S/C9H6F3N/c10-9(11,12)8-3-1-2-7(6-8)4-5-13/h1-3,6H,4H2
InchiKey:	JOIYKSLWXLFGGR-UHFFFAOYSA-N
Formula:	C9H6F3N
SMILES:	N#CCc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	185.15
CAS:	2338-76-3

Physical Properties

Property code	Value	Unit	Source
gf	-320.73	kJ/mol	Joback Method
hf	-436.23	kJ/mol	Joback Method
hfus	16.05	kJ/mol	Joback Method
hvap	45.30	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.771		Crippen Method
mcvol	120.600	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
tb	533.64	K	Joback Method
tc	742.11	K	Joback Method
tf	299.31	K	Joback Method
vc	0.500	m3/kmol	Joback Method

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	365.70	K	0.50	NIST Webbook
tbrp	365.50 ± 0.50	K	0.50	NIST Webbook

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=C2338763&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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