

Trifluoromethylisocyanide

Inchi:	InChI=1S/C2F3N/c1-6-2(3,4)5
InchiKey:	LKHQVUSYAMWNQZ-UHFFFAOYSA-N
Formula:	C2F3N
SMILES:	[C-]#[N+]C(F)(F)F
Mol. weight [g/mol]:	95.02
CAS:	105879-13-8

Physical Properties

Property code	Value	Unit	Source
gf	-482.45	kJ/mol	Joback Method
hf	-417.00 ± 29.00	kJ/mol	NIST Webbook
hfus	4.27	kJ/mol	Joback Method
hvap	26.78	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	1.425		Crippen Method
mcvol	45.730	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
tb	341.82	K	Joback Method
tc	516.00	K	Joback Method
tf	181.48	K	Joback Method
vc	0.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	82.59	J/molxK	341.82	Joback Method
cpg	86.37	J/molxK	370.85	Joback Method
cpg	89.86	J/molxK	399.88	Joback Method
cpg	93.07	J/molxK	428.91	Joback Method
cpg	96.03	J/molxK	457.94	Joback Method
cpg	98.75	J/molxK	486.97	Joback Method
cpg	101.24	J/molxK	516.00	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=C105879138&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

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