

C10HF7N2

Inchi:	InChI=1S/C10HF7N2/c11-6-4(3(1-18)2-19)7(12)9(14)5(8(6)13)10(15,16)17/h3H
InchiKey:	IQOLPUUIUYCGTI-UHFFFAOYSA-N
Formula:	C10HF7N2
SMILES:	N#CC(C#N)c1c(F)c(F)c(C(F)(F)F)c(F)c1F
Mol. weight [g/mol]:	282.12
CAS:	55852-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-999.33	kJ/mol	Joback Method
hf	-1127.59	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.393		Crippen Method
mcvol	143.150	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
tb	675.16	K	Joback Method
tc	867.69	K	Joback Method
tf	413.01	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.83	J/mol×K	675.16	Joback Method
cpg	365.27	J/mol×K	707.25	Joback Method
cpg	371.26	J/mol×K	739.34	Joback Method
cpg	376.82	J/mol×K	771.42	Joback Method
cpg	381.98	J/mol×K	803.51	Joback Method
cpg	386.75	J/mol×K	835.60	Joback Method
cpg	391.16	J/mol×K	867.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C55852249&Units=SI

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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