

3-Trifluoromethylbenzoylacetonitrile

Inchi:	InChI=1S/C10H6F3NO/c11-10(12,13)8-3-1-2-7(6-8)9(15)4-5-14/h1-3,6H,4H2
InchiKey:	GEPORLBYZLQDOB-UHFFFAOYSA-N
Formula:	C10H6F3NO
SMILES:	N#CCC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	213.16
CAS:	27328-86-5

Physical Properties

Property code	Value	Unit	Source
gf	-441.23	kJ/mol	Joback Method
hf	-569.45	kJ/mol	Joback Method
hfus	20.24	kJ/mol	Joback Method
hvap	54.27	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.802		Crippen Method
mvol	136.260	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	610.39	K	Joback Method
tc	823.29	K	Joback Method
tf	360.51	K	Joback Method
vc	0.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.62	J/mol×K	610.39	Joback Method
cpg	338.38	J/mol×K	645.87	Joback Method
cpg	347.37	J/mol×K	681.36	Joback Method
cpg	355.64	J/mol×K	716.84	Joback Method
cpg	363.25	J/mol×K	752.33	Joback Method
cpg	370.24	J/mol×K	787.81	Joback Method
cpg	376.66	J/mol×K	823.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27328865&Units=SI
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

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
mccvol:	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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