3-Trifluoromethyl-«alpha»,«alpha»,«alpha»-trifluo

Other names: 3-Trifluoromethyltrifluoroacetophenone
Inchi: InChI=1S/C9H4F6O/c10-8(11,12)6-3-1-2-5(4-6)7(16)9(13,14)15/h1-4H
InchiKey: MDCHHRZBYSSONX-UHFFFAOYSA-N
Formula: C9H4F6O
SMILES: O=C(c1cccc(C(F)(F)F)c1)C(F)(F)F
Mol. weight [g/mol]: 242.12
CAS: 721-37-9

Physical Properties

Property code	Value	Unit	Source
gf	-1164.42	kJ/mol	Joback Method
hf	-1310.77	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	37.82	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.450		Crippen Method
mcvol	126.100	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	480.01	K	Joback Method
tc	662.14	K	Joback Method
tf	288.44	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.87	J/mol×K	480.01	Joback Method
cpg	300.94	J/mol×K	510.37	Joback Method
cpg	311.18	J/mol×K	540.72	Joback Method
cpg	320.64	J/mol×K	571.08	Joback Method
cpg	329.37	J/mol×K	601.43	Joback Method
cpg	337.41	J/mol×K	631.79	Joback Method
cpg	344.79	J/mol×K	662.14	Joback Method

Sources

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=C721379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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