3',5'-BIS(TRIFLUOROMETHYL)ACETOPHENONE

Other names:	3,5-Bis(trifluoromethyl)acetophenone
	3,5-di(Trifluoromethyl)acetophenone
	Ethanone, 1-[3,5-bis(trifluoromethyl)phenyl]-
	1-[3,5-bis(trifluoromethyl)phenyl]ethan-1-one
Inchi:	InChI=1S/C10H6F6O/c1-5(17)6-2-7(9(11,12)13)4-8(3-6)10(14,15)16/h2-4H,1H3
InchiKey:	MCYCSIKSZLARBD-UHFFFAOYSA-N
Formula:	C10H6F6O
SMILES:	CC(=O)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	256.14

Physical Properties

Property code	Value	Unit	Source
ea	1.15 ± 0.09	eV	NIST Webbook
ea	1.12 ± 0.09	eV	NIST Webbook
hf	-1398.36	kJ/mol	Cheméo Relay (1.0)
hfus	20.17	kJ/mol	Joback Method
ie	9.90	eV	Cheméo Relay (1.0)
logp	3.927		Crippen Method
mcvol	140.190	ml/mol	McGowan Method
tb	463.49	K	Cheméo Relay (1.0)
tf	374.74	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.05	J/mol×K	507.87	Joback Method
cpg	344.47	J/mol×K	538.11	Joback Method
cpg	355.10	J/mol×K	568.35	Joback Method
cpg	364.98	J/mol×K	598.59	Joback Method
cpg	374.15	J/mol×K	628.83	Joback Method
cpg	382.65	J/mol×K	659.08	Joback Method
cpg	390.52	J/mol×K	689.32	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30071933&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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