4-TRIFLUOROMETHYL-BENZALACETONE

Other names:	p-Trifluoromethylbenzalacetone
	Z)-4(4-Trifluoromethylphenyl)-but-3-en-2-one
	4-Trifluoromethyl-benzalacetone
Inchi:	InChI=1S/C11H9F3O/c1-8(15)2-3-9-4-6-10(7-5-9)11(12,13)14/h2-7H,1H3/b3-2+
InchiKey:	PHVQEHOBDSECPV-NSCUHMNNSA-N
Formula:	C11H9F3O
SMILES:	CC(=O)/C=C\c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	214.19

Physical Properties

Property code	Value	Unit	Source
hf	-707.33	kJ/mol	Cheméo Relay (1.0)
hfus	21.53	kJ/mol	Joback Method
ie	9.12	eV	Cheméo Relay (1.0)
logp	3.308		Crippen Method
mcvol	144.670	ml/mol	McGowan Method
tb	508.89	K	Cheméo Relay (1.0)
tf	339.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.22	J/mol×K	535.35	Joback Method
cpg	344.05	J/mol×K	569.22	Joback Method
cpg	355.96	J/mol×K	603.08	Joback Method
cpg	367.00	J/mol×K	636.95	Joback Method
cpg	377.24	J/mol×K	670.81	Joback Method
cpg	386.72	J/mol×K	704.68	Joback Method
cpg	395.52	J/mol×K	738.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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?Str2File=C80992934
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
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