1,3-Butanedione, 4,4,4-trifluoro-1-phenyl-

Other names:	«omega»-(Trifluoroacetyl)acetophenone
	Benzoyl(trifluoroacetyl)methane
	1-Benzoyl-3,3,3-trifluoroacetone
	3-Benzoyl-1,1,1-trifluoroacetone
	4,4,4-Trifluoro-1-phenyl-1,3-butanedione
	Benzoyl-1,1,1-trifluoroacetone
	1-Benzoyl-3,3,3-trifluoro-2-propanone
	1,1,1-Trifluoro-4-phenyl-2,4-butanedione
	1-Phenyl-4,4,4-trifluoro-1,3-butanedione
	4-Phenyl-1,1,1-trifluorobutane-2,4-dione
	4,4,4-Trifluoro-1-phenyl-butane-1,3-dione
	BTA
	NSC 42628
Inchi:	InChI=1S/C10H7F3O2/c11-10(12,13)9(15)6-8(14)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	VVXLFFIFNVKFBD-UHFFFAOYSA-N
Formula:	C10H7F3O2
SMILES:	O=C(CC(=O)C(F)(F)F)c1ccccc1
Mol. weight [g/mol]:	216.16
CAS:	326-06-7

Physical Properties

Property code	Value	Unit	Source
chs	-4520.80 ± 3.40	kJ/mol	NIST Webbook
gf	-693.70	kJ/mol	Joback Method
hf	-865.60 ± 4.20	kJ/mol	NIST Webbook
hf	-875.20	kJ/mol	NIST Webbook
hf	-865.20	kJ/mol	NIST Webbook
hfs	-952.70 ± 4.10	kJ/mol	NIST Webbook
hfus	20.72	kJ/mol	Joback Method
hsub	87.09 ± 0.89	kJ/mol	NIST Webbook
hsub	77.50	kJ/mol	NIST Webbook
hsub	87.10 ± 0.90	kJ/mol	NIST Webbook
hvap	49.88	kJ/mol	Joback Method
ie	9.03	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.391		Crippen Method
mcvol	136.450	ml/mol	McGowan Method

pc	2963.34	kPa	Joback Method
tb	497.20	K	NIST Webbook
tc	761.86	K	Joback Method
tf	332.93	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.60	J/mol×K	557.20	Joback Method
cpg	333.12	J/mol×K	591.31	Joback Method
cpg	343.78	J/mol×K	625.42	Joback Method
cpg	353.61	J/mol×K	659.53	Joback Method
cpg	362.67	J/mol×K	693.64	Joback Method
cpg	371.01	J/mol×K	727.75	Joback Method
cpg	378.67	J/mol×K	761.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.00	K	0.70	NIST Webbook

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=C326067&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume