

3-Buten-2-one, 4-(3-trifluoromethylphenyl)-

Other names:	m-Trifluoromethylbenzalacetone 4-(3-Trifluoromethylphenyl)-3-buten-2-one Z)-4-(3-Trifluoromethylphenyl)-but-3-en-2-one 3-Trifluoromethyl-benzalacetone
Inchi:	InChI=1S/C11H9F3O/c1-8(15)5-6-9-3-2-4-10(7-9)11(12,13)14/h2-7H,1H3/b6-5+
InchiKey:	WIFIQCQDQCBMCM-AATRIKPKSA-N
Formula:	C11H9F3O
SMILES:	<chem>CC(=O)C=Cc1cccc(C(F)(F)F)c1</chem>
Mol. weight [g/mol]:	214.18
CAS:	80992-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-485.77	kJ/mol	Joback Method
hf	-637.75	kJ/mol	Joback Method
hfus	21.53	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
ie	9.10 ± 0.05	eV	NIST Webbook
log10ws	-3.52		Crippen Method
logp	3.308		Crippen Method
mcvol	144.670	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	535.35	K	Joback Method
tc	738.54	K	Joback Method
tf	301.71	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

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:	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=C80992923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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