2-(Trifluoromethyl)benzoyl chloride

Other names: 2-(Trifluoromethyl)benzoyl chloride
Inchi: InChI=1S/C8H4ClF3O/c9-7(13)5-3-1-2-4-6(5)8(10,11)12/h1-4H
InchiKey: MXIUWSYTQJLIKE-UHFFFAOYSA-N
Formula: C8H4ClF3O
SMILES: O=C(Cl)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 208.57

Physical Properties

Property code	Value	Unit	Source
hfus	17.75	kJ/mol	Joback Method
hvap	53.82	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-2.83		Cheméo Relay (1.0)
logp	3.084		Crippen Method
mcvol	118.940	ml/mol	McGowan Method
tb	457.65	K	Cheméo Relay (1.0)
tf	235.89	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.85	J/mol×K	499.98	Joback Method
cpg	254.75	J/mol×K	534.65	Joback Method
cpg	263.88	J/mol×K	569.32	Joback Method
cpg	272.28	J/mol×K	603.99	Joback Method
cpg	280.00	J/mol×K	638.66	Joback Method
cpg	287.08	J/mol×K	673.33	Joback Method
cpg	293.57	J/mol×K	708.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.00	K	2.10	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C312947&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point