Methyl 2-(N-trifluoroacetylamino)benzoate

Inchi: InChI=1S/C10H8F3NO3/c1-17-8(15)6-4-2-3-5-7(6)14-9(16)10(11,12)13/h2-5H,1H3,(H,14
InchiKey: UDEDDHDBRSUZQD-UHFFFAOYSA-N
Formula: C10H8F3NO3
SMILES: COC(=O)c1ccccc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 247.17

Physical Properties

Property code	Value	Unit	Source
gf	-718.94	kJ/mol	Joback Method
hf	-925.66	kJ/mol	Joback Method
hfus	26.62	kJ/mol	Joback Method
hvap	59.38	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	1.974		Crippen Method
mcvol	152.300	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1416.00		NIST Webbook
rinpol	1416.00		NIST Webbook
tb	634.77	K	Joback Method
tc	838.61	K	Joback Method
tf	420.34	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.09	J/mol×K	634.77	Joback Method
cpg	400.83	J/mol×K	668.74	Joback Method
cpg	410.79	J/mol×K	702.72	Joback Method
cpg	420.01	J/mol×K	736.69	Joback Method
cpg	428.52	J/mol×K	770.67	Joback Method
cpg	436.34	J/mol×K	804.64	Joback Method
cpg	443.53	J/mol×K	838.61	Joback Method

Sources

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=U374368&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume