4-(Trifluoroacetyl)benzoic acid

Inchi: InChI=1S/C9H5F3O3/c10-9(11,12)7(13)5-1-3-6(4-2-5)8(14)15/h1-4H,(H,14,15)
InchiKey: WLTZCRCZDLLXQP-UHFFFAOYSA-N
Formula: C9H5F3O3
SMILES: O=C(O)c1ccc(C(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 218.13
CAS: 58808-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-848.57	kJ/mol	Joback Method
hf	-978.50	kJ/mol	Joback Method
hfus	21.83	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.130		Crippen Method
mcvol	128.230	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	631.48	K	Joback Method
tc	827.15	K	Joback Method
tf	395.00	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.49	J/mol×K	631.48	Joback Method
cpg	327.58	J/mol×K	664.09	Joback Method
cpg	335.05	J/mol×K	696.70	Joback Method
cpg	341.94	J/mol×K	729.31	Joback Method
cpg	348.28	J/mol×K	761.92	Joback Method
cpg	354.11	J/mol×K	794.53	Joback Method
cpg	359.47	J/mol×K	827.15	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=C58808596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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