Acetanilide, 3-trifluoromethyl, acetoxy-M

Inchi: InChI=1S/C11H10F3NO3/c1-6(16)15-8-3-4-10(18-7(2)17)9(5-8)11(12,13)14/h3-5H,1-2H3
InchiKey: MCLKOUJVUAKQDM-UHFFFAOYSA-N
Formula: C11H10F3NO3
SMILES: CC(=O)Nc1ccc(OC(C)=O)c(C(F)(F)F)c1
Mol. weight [g/mol]: 261.20

Physical Properties

Property code	Value	Unit	Source
gf	-720.15	kJ/mol	Joback Method
hf	-957.77	kJ/mol	Joback Method
hfus	28.82	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.589		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1840.00		NIST Webbook
rinpol	1840.00		NIST Webbook
tb	662.63	K	Joback Method
tc	864.59	K	Joback Method
tf	444.13	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.65	J/mol×K	662.63	Joback Method
cpg	448.82	J/mol×K	696.29	Joback Method
cpg	459.23	J/mol×K	729.95	Joback Method
cpg	468.90	J/mol×K	763.61	Joback Method
cpg	477.86	J/mol×K	797.27	Joback Method
cpg	486.13	J/mol×K	830.93	Joback Method
cpg	493.75	J/mol×K	864.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R404369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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