2-Methoxy-5-nitrophenol, trifluoroacetate

Inchi: InChI=1S/C9H6F3NO5/c1-17-6-3-2-5(13(15)16)4-7(6)18-8(14)9(10,11)12/h2-4H,1H3
InchiKey: QVXOPRLVAGXWQE-UHFFFAOYSA-N
Formula: C9H6F3NO5
SMILES: COc1ccc([N+](=O)[O-])cc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 265.14

Physical Properties

Property code	Value	Unit	Source
gf	-766.91	kJ/mol	Joback Method
hf	-1000.36	kJ/mol	Joback Method
hfus	29.49	kJ/mol	Joback Method
hvap	63.64	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.071		Crippen Method
mcvol	149.950	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook
tb	687.09	K	Joback Method
tc	908.26	K	Joback Method
tf	484.84	K	Joback Method
vc	0.599	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.00	J/mol×K	687.09	Joback Method
cpg	404.73	J/mol×K	723.95	Joback Method
cpg	413.67	J/mol×K	760.81	Joback Method
cpg	421.85	J/mol×K	797.68	Joback Method
cpg	429.29	J/mol×K	834.54	Joback Method
cpg	436.00	J/mol×K	871.40	Joback Method
cpg	442.00	J/mol×K	908.26	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=U375943&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