2-Methoxy-5-nitrophenol, pentafluoropropionate

Inchi: InChI=1S/C10H6F5NO5/c1-20-6-3-2-5(16(18)19)4-7(6)21-8(17)9(11,12)10(13,14)15/h2-4

InchiKey: WCHCTHAWEVUBAN-UHFFFAOYSA-N

Formula: C10H6F5NO5

SMILES: COc1ccc([N+](=O)[O-])cc1OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 315.15

Physical Properties

Property code	Value	Unit	Source
gf	-1145.27	kJ/mol	Joback Method
hf	-1421.97	kJ/mol	Joback Method
hfus	30.83	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.706		Crippen Method
mcvol	167.580	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
tb	705.28	K	Joback Method
tc	916.13	K	Joback Method
tf	499.71	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.56	J/mol×K	705.28	Joback Method
cpg	473.15	J/mol×K	740.42	Joback Method
cpg	481.91	J/mol×K	775.56	Joback Method
cpg	489.90	J/mol×K	810.70	Joback Method
cpg	497.14	J/mol×K	845.85	Joback Method
cpg	503.68	J/mol×K	880.99	Joback Method
cpg	509.56	J/mol×K	916.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375942&Units=SI

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