2-Methoxy-5-nitrophenol, heptafluorobutyrate

Inchi: InChI=1S/C11H6F7NO5/c1-23-6-3-2-5(19(21)22)4-7(6)24-8(20)9(12,13)10(14,15)11(16,1

InchiKey: TZMZMRRWKKFFKQ-UHFFFAOYSA-N

Formula: C11H6F7NO5

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

Mol. weight [g/mol]: 365.16

Physical Properties

Property code	Value	Unit	Source
gf	-1523.63	kJ/mol	Joback Method
hf	-1843.58	kJ/mol	Joback Method
hfus	32.16	kJ/mol	Joback Method
hvap	62.23	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.342		Crippen Method
mcvol	185.210	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	723.47	K	Joback Method
tc	925.70	K	Joback Method
tf	514.58	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.66	J/mol×K	723.47	Joback Method
cpg	542.03	J/mol×K	757.18	Joback Method
cpg	550.57	J/mol×K	790.88	Joback Method
cpg	558.33	J/mol×K	824.59	Joback Method
cpg	565.37	J/mol×K	858.29	Joback Method
cpg	571.74	J/mol×K	892.00	Joback Method
cpg	577.51	J/mol×K	925.70	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=U375941&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