m-Methoxybenzoic acid, 5-fluoro-2-nitrophenyl ester

Inchi: InChI=1S/C14H10FNO5/c1-20-11-4-2-3-9(7-11)14(17)21-13-8-10(15)5-6-12(13)16(18)19

InchiKey: QSNRNPKLPYXYKT-UHFFFAOYSA-N

Formula: C14H10FNO5

SMILES: COc1cccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])c1

Mol. weight [g/mol]: 291.23

Physical Properties

Property code	Value	Unit	Source
gf	-235.25	kJ/mol	Joback Method
hf	-477.53	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	80.64	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	2.962		Crippen Method
mcvol	193.100	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	837.84	K	Joback Method
tc	1086.14	K	Joback Method
tf	576.53	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.22	J/mol×K	837.84	Joback Method
cpg	550.03	J/mol×K	879.22	Joback Method
cpg	559.64	J/mol×K	920.61	Joback Method
cpg	568.05	J/mol×K	961.99	Joback Method
cpg	575.30	J/mol×K	1003.37	Joback Method
cpg	581.39	J/mol×K	1044.75	Joback Method
cpg	586.33	J/mol×K	1086.14	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=U292632&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