p-Toluic acid, 5-fluoro-2-nitrophenyl ester

Other names: p-Toluylic acid, 5-fluoro-2-nitrophenyl ester
Inchi: InChI=1S/C14H10FNO4/c1-9-2-4-10(5-3-9)14(17)20-13-8-11(15)6-7-12(13)16(18)19/h2-
InchiKey: YFLLWSACVUSIJM-UHFFFAOYSA-N
Formula: C14H10FNO4
SMILES: Cc1ccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])cc1
Mol. weight [g/mol]: 275.23

Physical Properties

Property code	Value	Unit	Source
gf	-130.25	kJ/mol	Joback Method
hf	-345.31	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	78.23	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.262		Crippen Method
mcvol	187.230	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1956.60		NIST Webbook
tb	815.42	K	Joback Method
tc	1067.37	K	Joback Method
tf	554.30	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.80	J/mol×K	815.42	Joback Method
cpg	526.11	J/mol×K	857.41	Joback Method
cpg	536.29	J/mol×K	899.40	Joback Method
cpg	545.36	J/mol×K	941.40	Joback Method
cpg	553.37	J/mol×K	983.39	Joback Method
cpg	560.35	J/mol×K	1025.38	Joback Method
cpg	566.37	J/mol×K	1067.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292646&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