4-Cyanobenzoic acid, 5-fluoro-2-nitrophenyl ester

Inchi: InChI=1S/C14H7FN2O4/c15-11-5-6-12(17(19)20)13(7-11)21-14(18)10-3-1-9(8-16)2-4-10

InchiKey: VQTYKYJPTZOPLV-UHFFFAOYSA-N

Formula: C14H7FN2O4

SMILES: N#Cc1ccc(C(=O)Oc2cc(F)ccc2[N+](=O)[O-])cc1

Mol. weight [g/mol]: 286.21

Physical Properties

Property code	Value	Unit	Source
gf	2.93	kJ/mol	Joback Method
hf	-180.43	kJ/mol	Joback Method
hfus	37.66	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	2.825		Crippen Method
mcvol	188.610	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	2247.70		NIST Webbook
rinpol	2247.70		NIST Webbook
tb	917.50	K	Joback Method
tc	1177.77	K	Joback Method
tf	619.29	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.72	J/mol×K	917.50	Joback Method
cpg	526.57	J/mol×K	960.88	Joback Method
cpg	533.35	J/mol×K	1004.26	Joback Method
cpg	539.11	J/mol×K	1047.63	Joback Method
cpg	543.90	J/mol×K	1091.01	Joback Method
cpg	547.75	J/mol×K	1134.39	Joback Method
cpg	550.71	J/mol×K	1177.77	Joback Method

Sources

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=U292661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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