3-Nitrophenol, pentafluoropropionate

Inchi: InChI=1S/C9H4F5NO4/c10-8(11,9(12,13)14)7(16)19-6-3-1-2-5(4-6)15(17)18/h1-4H
InchiKey: QLUMEWYWOFNXRJ-UHFFFAOYSA-N
Formula: C9H4F5NO4
SMILES: O=C(Oc1cccc([N+](=O)[O-])c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 285.12

Physical Properties

Property code	Value	Unit	Source
gf	-1039.06	kJ/mol	Joback Method
hf	-1257.64	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	2.698		Crippen Method
mcvol	147.620	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
tb	655.00	K	Joback Method
tc	870.50	K	Joback Method
tf	453.69	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.58	J/mol×K	655.00	Joback Method
cpg	402.97	J/mol×K	690.92	Joback Method
cpg	411.49	J/mol×K	726.83	Joback Method
cpg	419.19	J/mol×K	762.75	Joback Method
cpg	426.14	J/mol×K	798.67	Joback Method
cpg	432.40	J/mol×K	834.58	Joback Method
cpg	438.03	J/mol×K	870.50	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=U375687&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