3-Nitrophenol, heptafluorobutyrate

Inchi: InChI=1S/C10H4F7NO4/c11-8(12,9(13,14)10(15,16)17)7(19)22-6-3-1-2-5(4-6)18(20)21/h
InchiKey: AVFHBJSMSJZVFE-UHFFFAOYSA-N
Formula: C10H4F7NO4
SMILES: O=C(Oc1cccc([N+](=O)[O-])c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 335.13

Physical Properties

Property code	Value	Unit	Source
gf	-1417.42	kJ/mol	Joback Method
hf	-1679.25	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	56.93	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.333		Crippen Method
mcvol	165.250	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1283.00		NIST Webbook
tb	673.19	K	Joback Method
tc	878.53	K	Joback Method
tf	468.56	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.39	J/mol×K	673.19	Joback Method
cpg	470.70	J/mol×K	707.41	Joback Method
cpg	479.11	J/mol×K	741.64	Joback Method
cpg	486.69	J/mol×K	775.86	Joback Method
cpg	493.52	J/mol×K	810.08	Joback Method
cpg	499.68	J/mol×K	844.30	Joback Method
cpg	505.24	J/mol×K	878.53	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=U375686&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