2-Nitrophenol, O-trifluoroacetyl-

Inchi: InChI=1S/C8H4F3NO4/c9-8(10,11)7(13)16-6-4-2-1-3-5(6)12(14)15/h1-4H
InchiKey: VXBYODJVYJMASS-UHFFFAOYSA-N
Formula: C8H4F3NO4
SMILES: O=C(Oc1ccccc1[N+](=O)[O-])C(F)(F)F
Mol. weight [g/mol]: 235.12

Physical Properties

Property code	Value	Unit	Source
gf	-660.70	kJ/mol	Joback Method
hf	-836.03	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	58.34	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.062		Crippen Method
mcvol	129.990	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	1231.00		NIST Webbook
rinpol	1231.00		NIST Webbook
tb	636.81	K	Joback Method
tc	864.12	K	Joback Method
tf	438.82	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.53	J/mol×K	636.81	Joback Method
cpg	335.87	J/mol×K	674.70	Joback Method
cpg	344.39	J/mol×K	712.58	Joback Method
cpg	352.14	J/mol×K	750.47	Joback Method
cpg	359.16	J/mol×K	788.35	Joback Method
cpg	365.50	J/mol×K	826.24	Joback Method
cpg	371.18	J/mol×K	864.12	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=U374260&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

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