Acetic acid, trifluoro-, 4-nitrophenyl ester

Other names:	p-Nitrophenyl trifluoroacetate
	4-Nitrophenyl trifluoroacetate
	Acetic acid, trifluoro-, p-nitrophenyl ester
	Trifluoroacetic acid p-nitrophenyl ester
	Trifluoroacetic acid, 4-nitrophenyl ester
Inchi:	InChI=1S/C8H4F3NO4/c9-8(10,11)7(13)16-6-3-1-5(2-4-6)12(14)15/h1-4H
InchiKey:	JFOIBTLTZWOAIC-UHFFFAOYSA-N
Formula:	C8H4F3NO4
SMILES:	O=C(Oc1ccc([N+](=O)[O-])cc1)C(F)(F)F
Mol. weight [g/mol]:	235.12
CAS:	658-78-6

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	1240.00		NIST Webbook
rinpol	1188.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	1.60	NIST Webbook

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=C658786&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume