3-Trifluoromethylbenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C14H8F3NO4/c15-14(16,17)10-3-1-2-9(8-10)13(19)22-12-6-4-11(5-7-12)18(20

InchiKey: MPDUMTCMFAHNSU-UHFFFAOYSA-N

Formula: C14H8F3NO4

SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 311.21

Physical Properties

Property code	Value	Unit	Source
gf	-507.40	kJ/mol	Joback Method
hf	-734.81	kJ/mol	Joback Method
hfus	35.29	kJ/mol	Joback Method
hvap	74.63	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.833		Crippen Method
mcvol	190.770	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	2016.00		NIST Webbook
rinpol	2016.00		NIST Webbook
tb	805.75	K	Joback Method
tc	1049.32	K	Joback Method
tf	545.38	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.88	J/mol×K	805.75	Joback Method
cpg	544.34	J/mol×K	846.35	Joback Method
cpg	553.72	J/mol×K	886.94	Joback Method
cpg	562.12	J/mol×K	927.54	Joback Method
cpg	569.61	J/mol×K	968.13	Joback Method
cpg	576.27	J/mol×K	1008.73	Joback Method
cpg	582.18	J/mol×K	1049.32	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=U307682&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