5-Nitrothiophene-2-carboxaldehyde

Other names:	2-Thiophenecarboxaldehyde, 5-nitro-
	5-Nitro 2-thiophenecarboxaldehyde
	5-Nitrothiophene-2-carboxaldehyde
	5-nitrothiophene-2-carbaldehyde
	Thiophenecarboxaldehyde, 5-nitro-
Inchi:	InChI=1S/C5H3NO3S/c7-3-4-1-2-5(10-4)6(8)9/h1-3H
InchiKey:	CHTSWZNXEKOLPM-UHFFFAOYSA-N
Formula:	C5H3NO3S
SMILES:	O=Cc1ccc([N+](=O)[O-])s1
Mol. weight [g/mol]:	157.15

Physical Properties

Property code	Value	Unit	Source
hvap	72.06	kJ/mol	Cheméo Relay (1.0)
logp	1.469		Crippen Method
mcvol	97.190	ml/mol	McGowan Method
tf	350.82	K	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521339&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point