7-Methyl-8-nitro-quinoline

Other names: Quinoline, 7-methyl-8-nitro-
8-Nitro-7-methylquinoline
Inchi: InChI=1S/C10H8N2O2/c1-7-4-5-8-3-2-6-11-9(8)10(7)12(13)14/h2-6H,1H3
InchiKey: ZZDTVYJYMRSNQL-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: Cc1ccc2cccnc2c1[N+](=O)[O-]
Mol. weight [g/mol]: 188.19

Physical Properties

Property code	Value	Unit	Source
af	0.5563		Cheméo Relay (1.0)
hf	155.42	kJ/mol	Cheméo Relay (1.0)
hvap	71.33	kJ/mol	Cheméo Relay (1.0)
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-2.99		Cheméo Relay (1.0)
logp	2.451		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3918.60	kPa	Cheméo Relay (1.0, beta)
rinpol	305.75		NIST Webbook
tb	597.20	K	Cheméo Relay (1.0)
tc	894.51	K	Cheméo Relay (1.0)
tf	358.28	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=C7471638&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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