Tranid

Other names: (6Z)-5-Chloro-6-{[(methylcarbamoyl)oxy]imino}bicyclo[2.2.1]heptane-2-carbonitrile

2-Norbornanecarbonitrile, 5-chloro-6-oxo-, O-(methylcarbamoyl)oxime, (E)-

2-Norbornanone, exo-3-chloro-endo-6-cyano-, O-(methylcarbamoyl)oxime, (E)-

3-Chloro-6-cyano-2-norbornanone-O-(methylcarbamoyl)oxime, 3-exo, 6-endo, (E)-

3-Chloro-6-cyanonorbornanone-2 oxime O,N-methylcarbamate

3-exo-Chloro-E-6-endo-cyano-2-norbornanone-O-(methylcarbamoyl)oxime

5-Chloro-6-((((methylamino)carbonyl)oxy)imino)bicyclo(2.2.1)heptane-2-carbonitrile, (1S-(1«alpha», 2«beta», 4«alpha», 5«alpha», 6E))-

5-Chloro-6-[[((methylamino)carbonyl)oxy]imino]bicyclo[2.2.1]heptane-2-carbonitrile, (1S-(1A«alpha»,2A«betaA»,4A«alpha»,5A«alpha»,6E))-

Bicyclo[2.2.1]heptane-2-carbonitrile, 5-chloro-6-[[[(methylamino)carbonyl]oxy]imino]-, (1S,2R,4R,5R,6E)-

Bicyclo[2.2.1]heptane-2-carbonitrile, 5-chloro-6-[[[(methylamino)carbonyl]oxy]imino]-, [1S-(1«alpha», 2«beta», 4«alpha», 5«alpha», 6E)]-

5-Chloro-6-[[(methylamino)carbonyl]oxy]imino]-, [1S-(1Â«alphaÂ»,2Â«betaÂ»,4Â«alphaÂ»,5Â«alphaÂ»,6E)]-

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exo-3-Chloro-endo-6-cyano-2-norbornanone O-(methylcarbamoyl)oxime

exo-5-Chloro-6-oxo-endo-2-norbornanecarbonitrile O-(methylcarbamoyl)oxime

Inchi: InChI=1S/C10H12ClN3O2/c1-13-10(15)16-14-9-7-3-5(8(9)11)2-6(7)4-12/h5-8H,2-3H2,1H

InchiKey: QCQPGRMMDFIQMB-UHFFFAOYSA-N

Formula: C10H12ClN3O2

SMILES: CNC(=O)ON=C1C(Cl)C2CC(C#N)C1C2

Mol. weight [g/mol]: 241.67

CAS: 15271-41-7

Physical Properties

Property code	Value	Unit	Source
hf	-152.13	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-2.08		Aqueous Solubility Prediction Method
logp	1.485		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
tb	781.74	K	Joback Method
tc	1014.71	K	Joback Method
tf	433.40 ± 0.20	K	NIST Webbook
tf	431.40 ± 0.20	K	NIST Webbook
tf	430.60 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.07	kJ/mol	431.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15271417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point