

Thiourea, 1-naphthalenyl-

Other names:

Urea, 1-(1-naphthyl)-2-thio-
«alpha»-Naphthylthiocarbamide
«alpha»-Naphthylthiourea
Alrato
Antu
Anturat
Bantu
Chemical 109
Dirax
Kripid
Krysid
N-1-Naphthylthiourea
Rattrack
Smeesana
U 5227
1-(1-Naphthyl)-2-thiourea
1-Naphthyl(2-thiourea)
1-Naphthylthiourea
«alpha»-Naphthothiurea
Kill kantz
Krysid PI
N-(1-Naphthyl)-2-thiourea
Rat-Tu
USAF EK-P-5976
1-Naftil-tiourea
1-Naftythioureum
1-Naphthyl-thioharnstoff
1-Naphthyl-thiouree
Alphanaphthyl thiourea
Alphanaphtyl thiouree
1-Naphthalenylthiourea
Naphtox
Rcra waste number P072
UN 1651
Thiourea, N-1-naphthalenyl-
1-(1-Naphthyl)thiourea
NSC 3287

Inchi: InChI=1S/C11H10N2S/c12-11(14)13-10-7-3-5-8-4-1-2-6-9(8)10/h1-7H,(H3,12,13,14)
InchiKey: PIVQQUNOTICCSA-UHFFFAOYSA-N
Formula: C11H10N2S

SMILES: N=C(S)Nc1cccc2ccccc12
Mol. weight [g/mol]: 202.28
CAS: 86-88-4

Physical Properties

Property code	Value	Unit	Source
gf	573.55	kJ/mol	Joback Method
hf	436.04	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.116		Crippen Method
mcvol	154.640	ml/mol	McGowan Method
tb	699.09	K	Joback Method
tf	443.27	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.92	J/mol×K	699.09	Joback Method
cpg	37.61	J/mol×K	100.12	Joback Method
cpg	37.61	J/mol×K	100.12	Joback Method
cpg	37.61	J/mol×K	100.12	Joback Method
cpg	37.61	J/mol×K	100.12	Joback Method
cpg	37.61	J/mol×K	100.12	Joback Method
cpg	37.61	J/mol×K	100.12	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=C86884&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
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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