Dipropetryn

Other names:	1,3,5-Triazine-2,4-diamine, 6-(ethylthio)-N,N'-bis(1-methylethyl)-
	s-Triazine, 2-(ethylthio)-4,6-bis(isopropylamino)-
	Cotofor
	GS 16068
	Sancap
	Dipropetryne
	s-Triazine, 2,4-bis(isopropylamino)-6-ethylthio-
	2-Ethylthio-4,6-bis(isopropylamino)-s-triazine
	6-(Ethylthio)-N,N'-bis(1-methylethyl)-1,3,5-triazine-2,4-diamine
Inchi:	InChI=1S/C11H21N5S/c1-6-17-11-15-9(12-7(2)3)14-10(16-11)13-8(4)5/h7-8H,6H2,1-5H3
InchiKey:	NPWMZOGDXOFZIN-UHFFFAOYSA-N
Formula:	C11H19N5S
SMILES:	CCSc1nc(=NC(C)C)[nH]c(=NC(C)C)[nH]1
Mol. weight [g/mol]:	253.37
CAS:	4147-51-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Crippen Method
logp	0.504		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
rinpol	1925.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tf	378.13 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	23.94	kJ/mol	377.70	NIST Webbook
hfust	23.94	kJ/mol	377.70	NIST Webbook
hfust	23.94	kJ/mol	377.70	NIST Webbook
hfust	23.94	kJ/mol	377.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4147517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point