

1,3,5-Triazine-2,4-diamine, 6-(ethylthio)-N,N'-bis(1-methylethyl)-

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: C11H21N5S
SMILES: CCSc1nc(NC(C)C)nc(NC(C)C)n1
Mol. weight [g/mol]: 255.39

Physical Properties

Property code	Value	Unit	Source
hf	-36.64	kJ/mol	Cheméo Relay (1.0)
hvap	115.55	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.33		Cheméo Relay (1.0)
logp	2.624		Crippen Method
mcvol	208.340	ml/mol	McGowan Method
tf	371.59	K	Cheméo Relay (1.0)

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
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=C4147517&Units=SI>

Legend

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

tf: Normal melting (fusion) point

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