Carbamothioic acid, cyclohexylethyl-, S-ethyl ester

Other names: Carbamic acid, cyclohexylethylthio-, S-ethyl ester
Cyclohexanecarbamic acid, N-ethylthio-, S-ethyl ester
Etsan
Eurex
Hexylthiocarbam
R 2063
Ro-Neet
Ro-Neet 6E
Ronit
S-Ethyl (cyclohexyl)ethylthiocarbamate
S-Ethyl N-cyclohexyl-N-ethylthiocarbamate
S-Ethyl N-ethyl-N-cyclohexylthiocarbamate
S-ethyl N-cyclohexylthiocarbamate
Sabet
cycloate

Inchi: InChI=1S/C11H21NOS/c1-3-12(11(13)14-4-2)10-8-6-5-7-9-10/h10H,3-9H2,1-2H3

InchiKey: DFCAFRGABIXSDS-UHFFFAOYSA-N

Formula: C11H21NOS

SMILES: CCSC(=O)N(CC)C1CCCCC1

Mol. weight [g/mol]: 215.36

Physical Properties

Property code	Value	Unit	Source
hfus	24.83	kJ/mol	Joback Method
log10ws	-3.40		Aqueous Solubility Prediction Method
log10ws	-3.40		Estimated Solubility Method
logp	3.514		Crippen Method
mcvol	182.890	ml/mol	McGowan Method
rinpol	1638.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	562.30	K	Cheméo Relay (1.0)
tf	284.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.17	J/mol×K	605.72	Joback Method
cpg	495.47	J/mol×K	642.28	Joback Method
cpg	513.55	J/mol×K	678.83	Joback Method
cpg	530.43	J/mol×K	715.39	Joback Method
cpg	546.17	J/mol×K	751.95	Joback Method
cpg	560.80	J/mol×K	788.51	Joback Method
cpg	574.35	J/mol×K	825.06	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134232&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point