Cycloate

Other names:	Carbamic acid, cyclohexylethylthio-, S-ethyl ester
	Carbamothioic acid, cyclohexylethyl-, 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
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
CAS:	1134-23-2

Physical Properties

Property code	Value	Unit	Source
gf	81.17	kJ/mol	Joback Method
hf	-219.23	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	56.11	kJ/mol	Joback Method
log10ws	-3.40		Estimated Solubility Method
log10ws	-3.40		Aqueous Solubility Prediction Method
logp	3.514		Crippen Method
mcvol	182.890	ml/mol	McGowan Method
pc	2522.65	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1642.00		NIST Webbook

tb	605.72	K	Joback Method
tc	825.06	K	Joback Method
tf	284.65	K	Aqueous Solubility Prediction Method
vc	0.662	m3/kmol	Joback 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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1134232&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
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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

pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume