Pebulate

Other names:	Butylethylthiocarbamic acid S-propyl ester
	Carbamic acid, butylethylthio-, S-propyl ester
	Carbamothioic acid, N-butyl-N-ethyl-, S-propyl ester
	Carbamothioic acid, butylethyl-, S-propyl ester
	PEBC
	Propyl N-ethyl-N-butylthiocarbamate
	Propyl ethylbutylthiolcarbamate
	Propyl-ethylbutylthiocarbamate
	Propylethyl-n-butylthiocarbamate
	R-2061
	S-(n-Propyl)-N-ethyl-N-n-butylthiocarbamate
	S-Propyl butylethylthiocarbamate
	S-Propyl-N-aethyl-N-butyl-thiocarbamat
	S-Propyl-N-butyl-N-ethylthiocarbamate
	S-Propyl-N-ethyl-N-butylthiocarbamate
	Stauffer R-2061
	Tillam
	Tillam-6-E
	n-Propyl N-ethyl-N-(n-butyl)thiocarbamate
	pedulate
Inchi:	InChI=1S/C10H21NOS/c1-4-7-8-11(6-3)10(12)13-9-5-2/h4-9H2,1-3H3
InchiKey:	SGEJQUSYQTVSIU-UHFFFAOYSA-N
Formula:	C10H21NOS
SMILES:	CCCCN(CC)C(=O)SCCC
Mol. weight [g/mol]:	203.34
CAS:	1114-71-2

Physical Properties

Property code	Value	Unit	Source
gf	48.30	kJ/mol	Joback Method
hf	-252.91	kJ/mol	Joback Method
hfus	30.41	kJ/mol	Joback Method
hvap	53.46	kJ/mol	Joback Method
log10ws	-3.53		Estimated Solubility Method
log10ws	-3.38		Aqueous Solubility Prediction Method

logp	3.372		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1472.00		NIST Webbook
tb	563.29	K	Joback Method
tc	751.85	K	Joback Method
tf	319.26	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.53	J/mol×K	563.29	Joback Method
cpg	450.89	J/mol×K	594.72	Joback Method
cpg	465.50	J/mol×K	626.14	Joback Method
cpg	479.38	J/mol×K	657.57	Joback Method
cpg	492.55	J/mol×K	689.00	Joback Method
cpg	505.03	J/mol×K	720.42	Joback Method
cpg	516.84	J/mol×K	751.85	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1114712&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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