Carbamothioic acid, dipropyl-, S-propyl ester

Other names:	Carbamic acid, dipropylthio-, S-propyl ester
	Dipropylthiocarbamic acid S-propyl ester
	PPTC
	Perbulate
	Propyl N,N-dipropylthiolcarbamate
	Propyl dipropylthiolcarbamate
	R-1607
	S-Propyl dipropylthiocarbamate
	Surpass
	Vanalate
	Vernam
	Vernam 7E
	Vernolate
	n-Propyl-di-n-propylthiolcarbamate
Inchi:	InChI=1S/C10H21NOS/c1-4-7-11(8-5-2)10(12)13-9-6-3/h4-9H2,1-3H3
InchiKey:	OKUGPJPKMAEJOE-UHFFFAOYSA-N
Formula:	C10H21NOS
SMILES:	CCCSC(=O)N(CCC)CCC
Mol. weight [g/mol]:	203.34
CAS:	1929-77-7

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	-3.30		Aqueous Solubility Prediction Method
logp	3.372		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1459.00		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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1929777&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