Propylcarbamate

Other names:	Carbamic acid, propyl ester
	n-Propyl carbamate
	Propyl urethane
	Propylester kyseliny karbaminove
Inchi:	InChI=1S/C4H9NO2/c1-2-3-7-4(5)6/h2-3H2,1H3,(H2,5,6)
InchiKey:	YNTOKMNHRPSGFU-UHFFFAOYSA-N
Formula:	C4H9NO2
SMILES:	CCCOC(=N)O
Mol. weight [g/mol]:	103.12
CAS:	627-12-3

Physical Properties

Property code	Value	Unit	Source
chs	-2307.70 ± 0.42	kJ/mol	NIST Webbook
gf	-55.42	kJ/mol	Joback Method
hf	-212.01	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	0.906		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
tb	489.86	K	Joback Method
tf	286.67	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.08	J/mol×K	489.86	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
cpg	52.61	J/mol×K	100.12	Joback Method
hvapt	61.60	kJ/mol	396.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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