Propamocarb

Other names: Carbamic acid, N-[3-(dimethylamino)propyl]-, propyl ester
propyl [3-(dimethylamino)propyl]carbamate
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Inchi: InChI=1S/C9H20N2O2/c1-4-8-13-9(12)10-6-5-7-11(2)3/h4-8H2,1-3H3,(H,10,12)

InchiKey: WZZLDXDUQPOXNW-UHFFFAOYSA-N

Formula: C9H20N2O2

SMILES: CCCOC(=O)NCCCN(C)C

Mol. weight [g/mol]: 188.27

CAS: 24579-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-8.85	kJ/mol	Joback Method
hf	-352.89	kJ/mol	Joback Method
hfus	29.97	kJ/mol	Joback Method
hvap	53.26	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.074		Crippen Method
mcvol	165.070	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1393.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	544.22	K	Joback Method
tc	718.89	K	Joback Method
tf	348.48	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.94	J/mol×K	544.22	Joback Method
cpg	422.11	J/mol×K	573.33	Joback Method
cpg	435.68	J/mol×K	602.44	Joback Method
cpg	448.65	J/mol×K	631.56	Joback Method

cpg	461.03	J/mol×K	660.67	Joback Method
cpg	472.84	J/mol×K	689.78	Joback Method
cpg	484.08	J/mol×K	718.89	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24579735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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