CARBAMIC ACID, PROPYL ESTER

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

Physical Properties

Property code	Value	Unit	Source
af	0.5742		Cheméo Relay (1.0)
hf	-502.54	kJ/mol	Cheméo Relay (1.0)
hfus	14.10	kJ/mol	Joback Method
hvap	47.55	kJ/mol	Cheméo Relay (1.0)
ie	10.08	eV	Cheméo Relay (1.0)
log10ws	-0.75		Cheméo Relay (1.0)
logp	0.492		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	422.59	K	Cheméo Relay (1.0)
tc	593.01	K	Cheméo Relay (1.0)
tf	217.41	K	Cheméo Relay (1.0)
vc	0.322	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.31	J/mol×K	439.74	Joback Method
cpg	180.30	J/mol×K	472.17	Joback Method
cpg	188.01	J/mol×K	504.60	Joback Method
cpg	195.44	J/mol×K	537.03	Joback Method
cpg	202.59	J/mol×K	569.46	Joback Method
cpg	209.45	J/mol×K	601.88	Joback Method
cpg	216.03	J/mol×K	634.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C627123
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume