Carbamic acid, n-(2-phenyl-2-propyl), methyl ester

Inchi: InChI=1S/C11H15NO2/c1-11(2,12-10(13)14-3)9-7-5-4-6-8-9/h4-8H,1-3H3,(H,12,13)
InchiKey: LBYIYEHNLLZCQC-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: COC(=O)NC(C)(C)c1ccccc1
Mol. weight [g/mol]: 193.24
CAS: 102414-20-0

Physical Properties

Property code	Value	Unit	Source
gf	12.46	kJ/mol	Joback Method
hf	-233.92	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.278		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	600.99	K	Joback Method
tc	822.79	K	Joback Method
tf	367.39	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.67	J/mol×K	600.99	Joback Method
cpg	414.69	J/mol×K	637.96	Joback Method
cpg	428.67	J/mol×K	674.92	Joback Method
cpg	441.65	J/mol×K	711.89	Joback Method
cpg	453.68	J/mol×K	748.86	Joback Method
cpg	464.81	J/mol×K	785.82	Joback Method
cpg	475.10	J/mol×K	822.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C102414200&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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