Carbanilic acid, n-pentyl ester

Inchi: InChI=1S/C12H17NO2/c1-2-3-7-10-15-12(14)13-11-8-5-4-6-9-11/h4-6,8-9H,2-3,7,10H2,1
InchiKey: BIYXGLPPMRDUNY-UHFFFAOYSA-N
Formula: C12H17NO2
SMILES: CCCCCOC(=O)Nc1ccccc1
Mol. weight [g/mol]: 207.27
CAS: 63075-06-9

Physical Properties

Property code	Value	Unit	Source
gf	18.04	kJ/mol	Joback Method
hf	-245.81	kJ/mol	Joback Method
hfus	28.76	kJ/mol	Joback Method
hvap	60.17	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.425		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	627.10	K	Joback Method
tc	833.14	K	Joback Method
tf	376.24	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.98	J/mol×K	627.10	Joback Method
cpg	460.85	J/mol×K	661.44	Joback Method
cpg	474.84	J/mol×K	695.78	Joback Method
cpg	487.97	J/mol×K	730.12	Joback Method
cpg	500.27	J/mol×K	764.46	Joback Method
cpg	511.77	J/mol×K	798.80	Joback Method
cpg	522.49	J/mol×K	833.14	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=C63075069&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume