Carbanilic acid, n-methyl, isopropyl ester

Inchi: InChI=1S/C11H15NO2/c1-9(2)14-11(13)12(3)10-7-5-4-6-8-10/h4-9H,1-3H3
InchiKey: OGQJEQNWJVFSGO-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CC(C)OC(=O)N(C)c1ccccc1
Mol. weight [g/mol]: 193.24
CAS: 3295-92-9

Physical Properties

Property code	Value	Unit	Source
gf	28.57	kJ/mol	Joback Method
hf	-216.39	kJ/mol	Joback Method
hfus	20.57	kJ/mol	Joback Method
hvap	53.17	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.668		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
tb	566.05	K	Joback Method
tc	776.78	K	Joback Method
tf	329.78	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.16	J/mol×K	566.05	Joback Method
cpg	397.56	J/mol×K	601.17	Joback Method
cpg	412.03	J/mol×K	636.29	Joback Method
cpg	425.60	J/mol×K	671.41	Joback Method
cpg	438.29	J/mol×K	706.53	Joback Method
cpg	450.14	J/mol×K	741.66	Joback Method
cpg	461.18	J/mol×K	776.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3295929&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