P-methoxy carbanilic acid, n-butyl ester

Inchi: InChI=1S/C12H17NO3/c1-3-4-9-16-12(14)13-10-5-7-11(15-2)8-6-10/h5-8H,3-4,9H2,1-2H
InchiKey: RICFGOZAGKHWPX-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 223.27
CAS: 91644-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-96.59	kJ/mol	Joback Method
hf	-389.50	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	3.044		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
tb	654.50	K	Joback Method
tc	859.45	K	Joback Method
tf	410.99	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.35	J/mol×K	654.50	Joback Method
cpg	485.73	J/mol×K	688.66	Joback Method
cpg	499.29	J/mol×K	722.82	Joback Method
cpg	512.04	J/mol×K	756.97	Joback Method
cpg	523.99	J/mol×K	791.13	Joback Method
cpg	535.13	J/mol×K	825.29	Joback Method
cpg	545.47	J/mol×K	859.45	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=C91644881&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

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