P-methoxy carbanilic acid, n-nonyl ester

Inchi: InChI=1S/C17H27NO3/c1-3-4-5-6-7-8-9-14-21-17(19)18-15-10-12-16(20-2)13-11-15/h10
InchiKey: RGNHAQORUPJGNE-UHFFFAOYSA-N
Formula: C17H27NO3
SMILES: CCCCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 293.40
CAS: 94907-38-7

Physical Properties

Property code	Value	Unit	Source
gf	-54.49	kJ/mol	Joback Method
hf	-492.70	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	74.38	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.994		Crippen Method
mcvol	249.920	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
tb	768.90	K	Joback Method
tc	964.70	K	Joback Method
tf	467.34	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.23	J/mol×K	768.90	Joback Method
cpg	759.54	J/mol×K	801.53	Joback Method
cpg	774.84	J/mol×K	834.17	Joback Method
cpg	789.16	J/mol×K	866.80	Joback Method
cpg	802.51	J/mol×K	899.43	Joback Method
cpg	814.90	J/mol×K	932.06	Joback Method
cpg	826.36	J/mol×K	964.70	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94907387&Units=SI

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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