P-methoxy carbanilic acid, n-dodecyl ester

Inchi: InChI=1S/C20H33NO3/c1-3-4-5-6-7-8-9-10-11-12-17-24-20(22)21-18-13-15-19(23-2)16-
InchiKey: QCJVRXWWZWPGIV-UHFFFAOYSA-N
Formula: C20H33NO3
SMILES: CCCCCCCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 335.48
CAS: 116373-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-29.23	kJ/mol	Joback Method
hf	-554.62	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	81.05	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	6.165		Crippen Method
mcvol	292.190	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
tb	837.54	K	Joback Method
tc	1034.30	K	Joback Method
tf	501.15	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.83	J/mol×K	837.54	Joback Method
cpg	935.89	J/mol×K	870.33	Joback Method
cpg	951.81	J/mol×K	903.13	Joback Method
cpg	966.62	J/mol×K	935.92	Joback Method
cpg	980.36	J/mol×K	968.71	Joback Method
cpg	993.05	J/mol×K	1001.50	Joback Method
cpg	1004.71	J/mol×K	1034.30	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=C116373207&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