P-methoxy carbanilic acid, n-octyl ester

Inchi: InChI=1S/C16H25NO3/c1-3-4-5-6-7-8-13-20-16(18)17-14-9-11-15(19-2)12-10-14/h9-12H
InchiKey: BTUZIUSTDKPFOM-UHFFFAOYSA-N
Formula: C16H25NO3
SMILES: CCCCCCCCOC(=O)Nc1ccc(OC)cc1
Mol. weight [g/mol]: 279.37
CAS: 93146-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-62.91	kJ/mol	Joback Method
hf	-472.06	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	72.15	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.604		Crippen Method
mcvol	235.830	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
tb	746.02	K	Joback Method
tc	942.70	K	Joback Method
tf	456.07	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.55	J/mol×K	746.02	Joback Method
cpg	702.58	J/mol×K	778.80	Joback Method
cpg	717.64	J/mol×K	811.58	Joback Method
cpg	731.74	J/mol×K	844.36	Joback Method
cpg	744.90	J/mol×K	877.14	Joback Method
cpg	757.13	J/mol×K	909.92	Joback Method
cpg	768.46	J/mol×K	942.70	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=C93146340&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