P-nitro carbanilic acid, n-dodecyl ester

Inchi: InChI=1S/C19H30N2O4/c1-2-3-4-5-6-7-8-9-10-11-16-25-19(22)20-17-12-14-18(15-13-17
InchiKey: BFPRVWDBEWSDMC-UHFFFAOYSA-N
Formula: C19H30N2O4
SMILES: CCCCCCCCCCCCOC(=O)Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 350.45
CAS: 94432-01-6

Physical Properties

Property code	Value	Unit	Source
gf	102.90	kJ/mol	Joback Method
hf	-412.52	kJ/mol	Joback Method
hfus	57.87	kJ/mol	Joback Method
hvap	93.01	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.064		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
tb	944.08	K	Joback Method
tc	1163.02	K	Joback Method
tf	611.26	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.24	J/mol×K	944.08	Joback Method
cpg	961.51	J/mol×K	980.57	Joback Method
cpg	974.62	J/mol×K	1017.06	Joback Method
cpg	986.62	J/mol×K	1053.55	Joback Method
cpg	997.56	J/mol×K	1090.04	Joback Method
cpg	1007.50	J/mol×K	1126.53	Joback Method
cpg	1016.50	J/mol×K	1163.02	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=C94432016&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