4-Nitrobenzoic acid, dodecyl ester

Other names: dodecyl 4-nitrobenzoate
Inchi: InChI=1S/C19H29NO4/c1-2-3-4-5-6-7-8-9-10-11-16-24-19(21)17-12-14-18(15-13-17)20(
InchiKey: NIXNCBRIBRCGQE-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 335.44
CAS: 35507-03-0

Physical Properties

Property code	Value	Unit	Source
gf	13.51	kJ/mol	Joback Method
hf	-465.99	kJ/mol	Joback Method
hfus	52.77	kJ/mol	Joback Method
hvap	86.57	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	5.673		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1404.84	kPa	Joback Method
rinpol	2536.00		NIST Webbook
rinpol	2546.00		NIST Webbook
rinpol	2521.00		NIST Webbook
rinpol	2509.00		NIST Webbook
rinpol	2509.00		NIST Webbook
rinpol	2550.00		NIST Webbook
ripol	3288.00		NIST Webbook
ripol	3326.00		NIST Webbook
ripol	3341.00		NIST Webbook
ripol	3288.00		NIST Webbook
ripol	3342.00		NIST Webbook
tb	893.91	K	Joback Method
tc	1108.13	K	Joback Method
tf	558.60	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.06	J/mol×K	893.91	Joback Method
cpg	905.19	J/mol×K	929.61	Joback Method
cpg	919.18	J/mol×K	965.32	Joback Method
cpg	932.09	J/mol×K	1001.02	Joback Method
cpg	943.96	J/mol×K	1036.72	Joback Method
cpg	954.84	J/mol×K	1072.42	Joback Method
cpg	964.77	J/mol×K	1108.13	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=C35507030&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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume