p-Nitrobenzoic acid, n-propyl ester

Other names:	Benzoic acid, p-nitro-, propyl ester
	Benzoic acid, 4-nitro-, propyl ester
	Propyl 4-nitrobenzoate
Inchi:	InChI=1S/C10H11NO4/c1-2-7-15-10(12)8-3-5-9(6-4-8)11(13)14/h3-6H,2,7H2,1H3
InchiKey:	KXUOYHZSTGGNCK-UHFFFAOYSA-N
Formula:	C10H11NO4
SMILES:	CCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	209.20
CAS:	94-22-4

Physical Properties

Property code	Value	Unit	Source
gf	-62.27	kJ/mol	Joback Method
hf	-280.23	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.162		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1594.00		NIST Webbook
rinpol	1636.00		NIST Webbook
ripol	2367.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2426.00		NIST Webbook
ripol	2414.00		NIST Webbook
tb	687.99	K	Joback Method
tc	925.31	K	Joback Method
tf	457.17	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.14	J/mol×K	687.99	Joback Method
cpg	407.29	J/mol×K	727.54	Joback Method
cpg	418.53	J/mol×K	767.10	Joback Method
cpg	428.88	J/mol×K	806.65	Joback Method
cpg	438.36	J/mol×K	846.20	Joback Method
cpg	446.99	J/mol×K	885.75	Joback Method
cpg	454.81	J/mol×K	925.31	Joback Method

Sources

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=C94224&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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