4-Nitrobenzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C18H25NO4/c1-2-3-4-5-6-7-8-9-10-15-23-18(20)16-11-13-17(14-12-16)19(21)
InchiKey: RUSWJAOVWKDAEP-MDZDMXLPSA-N
Formula: C18H25NO4
SMILES: CCCCCCCCC=CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
gf	85.31	kJ/mol	Joback Method
hf	-328.13	kJ/mol	Joback Method
hfus	50.38	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.058		Crippen Method
mcvol	261.280	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	2404.00		NIST Webbook
rinpol	2404.00		NIST Webbook
tb	875.19	K	Joback Method
tc	1094.65	K	Joback Method
tf	542.25	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.03	J/mol×K	875.19	Joback Method
cpg	818.58	J/mol×K	911.77	Joback Method
cpg	832.11	J/mol×K	948.34	Joback Method
cpg	844.66	J/mol×K	984.92	Joback Method
cpg	856.30	J/mol×K	1021.50	Joback Method
cpg	867.10	J/mol×K	1058.08	Joback Method
cpg	877.10	J/mol×K	1094.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299272&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume