4-Nitrobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H27NO4/c1-2-3-4-5-6-7-8-9-10-11-12-17-25-20(22)18-13-15-19(16-14-18)
InchiKey: PQFGHRHZXSJQKZ-UHFFFAOYSA-N
Formula: C20H27NO4
SMILES: CCCCCCCCCCC#CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
gf	224.73	kJ/mol	Joback Method
hf	-214.33	kJ/mol	Joback Method
hfus	58.48	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.286		Crippen Method
mcvol	285.160	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2577.00		NIST Webbook
rinpol	2577.00		NIST Webbook
tb	925.79	K	Joback Method
tc	1152.25	K	Joback Method
tf	675.97	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.65	J/mol×K	925.79	Joback Method
cpg	909.24	J/mol×K	963.53	Joback Method
cpg	922.64	J/mol×K	1001.28	Joback Method
cpg	934.92	J/mol×K	1039.02	Joback Method
cpg	946.11	J/mol×K	1076.76	Joback Method
cpg	956.28	J/mol×K	1114.50	Joback Method
cpg	965.47	J/mol×K	1152.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299273&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