Benzeneacetic acid, 4-nitro-, undec-2-en-1-yl ester

Inchi: InChI=1S/C19H27NO4/c1-2-3-4-5-6-7-8-9-10-15-24-19(21)16-17-11-13-18(14-12-17)20(

InchiKey: DDQCNHRGXYOSBK-MDZDMXLPSA-N

Formula: C19H27NO4

SMILES: CCCCCCCCC=CCOC(=O)Cc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
gf	93.73	kJ/mol	Joback Method
hf	-348.77	kJ/mol	Joback Method
hfus	52.97	kJ/mol	Joback Method
hvap	86.53	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.987		Crippen Method
mcvol	275.370	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	898.07	K	Joback Method
tc	1116.83	K	Joback Method
tf	553.52	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.41	J/mol×K	898.07	Joback Method
cpg	877.19	J/mol×K	934.53	Joback Method
cpg	890.93	J/mol×K	970.99	Joback Method
cpg	903.69	J/mol×K	1007.45	Joback Method
cpg	915.53	J/mol×K	1043.91	Joback Method
cpg	926.52	J/mol×K	1080.37	Joback Method
cpg	936.72	J/mol×K	1116.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406981&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