Benzeneacetic acid, 4-nitro-, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H21NO4/c1-3-4-5-6-7-13(2)21-16(18)12-14-8-10-15(11-9-14)17(19)20/h6-1

InchiKey: QLVJLOPSGSCVAP-VOTSOKGWSA-N

Formula: C16H21NO4

SMILES: CCCCC=CC(C)OC(=O)Cc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 291.34

Physical Properties

Property code	Value	Unit	Source
gf	66.03	kJ/mol	Joback Method
hf	-292.13	kJ/mol	Joback Method
hfus	41.67	kJ/mol	Joback Method
hvap	79.47	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.815		Crippen Method
mcvol	233.100	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	828.99	K	Joback Method
tc	1055.21	K	Joback Method
tf	504.71	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.33	J/mol×K	828.99	Joback Method
cpg	704.59	J/mol×K	866.69	Joback Method
cpg	717.79	J/mol×K	904.40	Joback Method
cpg	729.99	J/mol×K	942.10	Joback Method
cpg	741.25	J/mol×K	979.80	Joback Method
cpg	751.64	J/mol×K	1017.50	Joback Method
cpg	761.20	J/mol×K	1055.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406978&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

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

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