Benzoic acid, 4-nitro-, octyl ester

Other names: 4-Nitrobenzoic acid, octyl ester
octyl 4-nitrobenzoate
octyl p-nitrobenzoate
Inchi: InChI=1S/C15H21NO4/c1-2-3-4-5-6-7-12-20-15(17)13-8-10-14(11-9-13)16(18)19/h8-11H
InchiKey: WHZYPQVZYYTVFW-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: CCCCCCCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 279.33
CAS: 6500-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-20.17	kJ/mol	Joback Method
hf	-383.43	kJ/mol	Joback Method
hfus	42.41	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.112		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2121.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2140.00		NIST Webbook
ripol	2874.00		NIST Webbook
ripol	2874.00		NIST Webbook
ripol	2926.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2874.00		NIST Webbook
ripol	2910.00		NIST Webbook
tb	802.39	K	Joback Method
tc	1021.16	K	Joback Method
tf	513.52	K	Joback Method

vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.01	J/mol×K	802.39	Joback Method
cpg	674.29	J/mol×K	838.85	Joback Method
cpg	687.53	J/mol×K	875.31	Joback Method
cpg	699.75	J/mol×K	911.78	Joback Method
cpg	711.01	J/mol×K	948.24	Joback Method
cpg	721.32	J/mol×K	984.70	Joback Method
cpg	730.73	J/mol×K	1021.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6500501&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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