4-Nitrobenzoic acid, 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]: 279.34

Physical Properties

Property code	Value	Unit	Source
af	0.8968		Cheméo Relay (1.0)
hf	-431.74	kJ/mol	Cheméo Relay (1.0)
hfus	42.41	kJ/mol	Joback Method
hvap	100.53	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-5.42		Cheméo Relay (1.0)
logp	4.112		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2140.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2108.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2108.00		NIST Webbook
ripol	2874.00		NIST Webbook
ripol	2926.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2874.00		NIST Webbook
ripol	2911.00		NIST Webbook
ripol	2910.00		NIST Webbook
ripol	2874.00		NIST Webbook
tb	606.25	K	Cheméo Relay (1.0)
tc	845.24	K	Cheméo Relay (1.0)
tf	310.03	K	Cheméo Relay (1.0)

vc	0.823	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6500501&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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