Phthalic acid, 2-(4-nitrophenoxy)ethyl propyl ester

Inchi: InChI=1S/C19H19NO7/c1-2-11-26-18(21)16-5-3-4-6-17(16)19(22)27-13-12-25-15-9-7-14

InchiKey: MCZVCEYLIPOISG-UHFFFAOYSA-N

Formula: C19H19NO7

SMILES: CCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 373.36

Physical Properties

Property code	Value	Unit	Source
gf	-222.63	kJ/mol	Joback Method
hf	-617.95	kJ/mol	Joback Method
hfus	50.39	kJ/mol	Joback Method
hvap	101.08	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.397		Crippen Method
mcvol	269.220	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	3327.00		NIST Webbook
rinpol	3327.00		NIST Webbook
tb	1024.28	K	Joback Method
tc	1269.52	K	Joback Method
tf	691.93	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.07	J/mol×K	1024.28	Joback Method
cpg	850.68	J/mol×K	1065.15	Joback Method
cpg	857.71	J/mol×K	1106.03	Joback Method
cpg	863.16	J/mol×K	1146.90	Joback Method
cpg	867.07	J/mol×K	1187.77	Joback Method
cpg	869.46	J/mol×K	1228.64	Joback Method
cpg	870.35	J/mol×K	1269.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382572&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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