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

Inchi: InChI=1S/C18H17NO7/c1-2-24-17(20)15-5-3-4-6-16(15)18(21)26-12-11-25-14-9-7-13(8-
InchiKey: YVCLFAWLRDETFF-UHFFFAOYSA-N
Formula: C18H17NO7
SMILES: CCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 359.33

Physical Properties

Property code	Value	Unit	Source
gf	-231.05	kJ/mol	Joback Method
hf	-597.31	kJ/mol	Joback Method
hfus	47.80	kJ/mol	Joback Method
hvap	98.85	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.007		Crippen Method
mcvol	255.130	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	3239.00		NIST Webbook
rinpol	3239.00		NIST Webbook
tb	1001.40	K	Joback Method
tc	1247.55	K	Joback Method
tf	680.66	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.93	J/mol×K	1001.40	Joback Method
cpg	793.60	J/mol×K	1042.43	Joback Method
cpg	800.73	J/mol×K	1083.45	Joback Method
cpg	806.31	J/mol×K	1124.48	Joback Method
cpg	810.38	J/mol×K	1165.50	Joback Method
cpg	812.94	J/mol×K	1206.53	Joback Method
cpg	814.01	J/mol×K	1247.55	Joback Method

Sources

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=U382571&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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