

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

Inchi:	InChI=1S/C19H19NO7/c1-2-11-26-18(21)14-3-5-15(6-4-14)19(22)27-13-12-25-17-9-7-16
InchiKey:	NCDRNUHRCVASAC-UHFFFAOYSA-N
Formula:	C19H19NO7
SMILES:	CCCOC(=O)c1ccc(C(=O)OCCOc2ccc([N+](=O)[O-])cc2)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	3236.00		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/molxK	1024.28	Joback Method
cpg	850.68	J/molxK	1065.15	Joback Method
cpg	857.71	J/molxK	1106.03	Joback Method
cpg	863.16	J/molxK	1146.90	Joback Method
cpg	867.07	J/molxK	1187.77	Joback Method
cpg	869.46	J/molxK	1228.64	Joback Method
cpg	870.35	J/molxK	1269.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416089&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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