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

Inchi: InChI=1S/C20H21NO7/c1-2-3-12-27-19(22)15-4-6-16(7-5-15)20(23)28-14-13-26-18-10-8

InchiKey: GYVFYHMXZVJTHB-UHFFFAOYSA-N

Formula: C20H21NO7

SMILES: CCCCOC(=O)c1ccc(C(=O)OCCOc2ccc([N+](=O)[O-])cc2)cc1

Mol. weight [g/mol]: 387.38

Physical Properties

Property code	Value	Unit	Source
gf	-214.21	kJ/mol	Joback Method
hf	-638.59	kJ/mol	Joback Method
hfus	52.98	kJ/mol	Joback Method
hvap	103.30	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	3.788		Crippen Method
mcvol	283.310	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
tb	1047.16	K	Joback Method
tc	1292.40	K	Joback Method
tf	703.20	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.67	J/mol×K	1047.16	Joback Method
cpg	908.19	J/mol×K	1088.03	Joback Method
cpg	915.08	J/mol×K	1128.91	Joback Method
cpg	920.37	J/mol×K	1169.78	Joback Method
cpg	924.08	J/mol×K	1210.65	Joback Method
cpg	926.25	J/mol×K	1251.53	Joback Method
cpg	926.89	J/mol×K	1292.40	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=U416091&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