

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

Inchi:	InChI=1S/C20H21NO7/c1-2-3-12-27-19(22)17-6-4-5-7-18(17)20(23)28-14-13-26-16-10-8
InchiKey:	CJLHBYZWCIBCJL-UHFFFAOYSA-N
Formula:	C20H21NO7
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCCOc1ccc([N+](=O)[O-])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
mvol	283.310	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
tb	1047.16	K	Joback Method
tc	1292.40	K	Joback Method
tf	703.20	K	Joback Method
vc	1.087	m ³ /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

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=U382574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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