Phthalic acid, heptyl 3-methoxy-4-nitrobenzyl ester

Inchi: InChI=1S/C23H27NO7/c1-3-4-5-6-9-14-30-22(25)18-10-7-8-11-19(18)23(26)31-16-17-12

InchiKey: ZOIFOVHYSWTNSU-UHFFFAOYSA-N

Formula: C23H27NO7

SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])c(OC)c1

Mol. weight [g/mol]: 429.46

Physical Properties

Property code	Value	Unit	Source
gf	-198.58	kJ/mol	Joback Method
hf	-711.98	kJ/mol	Joback Method
hfus	60.36	kJ/mol	Joback Method
hvap	110.64	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.088		Crippen Method
mcvol	325.580	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	3782.00		NIST Webbook
rinpol	3782.00		NIST Webbook
tb	1120.78	K	Joback Method
tc	1373.04	K	Joback Method
tf	749.53	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.58	J/mol×K	1120.78	Joback Method
cpg	1080.35	J/mol×K	1162.82	Joback Method
cpg	1086.24	J/mol×K	1204.87	Joback Method
cpg	1090.29	J/mol×K	1246.91	Joback Method
cpg	1092.52	J/mol×K	1288.95	Joback Method
cpg	1092.98	J/mol×K	1331.00	Joback Method
cpg	1091.70	J/mol×K	1373.04	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=U382535&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

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