Phthalic acid, heptyl 4-nitrobenzyl ester

Inchi: InChI=1S/C22H25NO6/c1-2-3-4-5-8-15-28-21(24)19-9-6-7-10-20(19)22(25)29-16-17-11-
InchiKey: IMIBRLSUNOVBIU-UHFFFAOYSA-N
Formula: C22H25NO6
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 399.44

Physical Properties

Property code	Value	Unit	Source
gf	-92.37	kJ/mol	Joback Method
hf	-547.65	kJ/mol	Joback Method
hfus	56.97	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	5.079		Crippen Method
mcvol	305.620	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	3655.00		NIST Webbook
rinpol	3655.00		NIST Webbook
tb	1070.50	K	Joback Method
tc	1316.39	K	Joback Method
tf	703.51	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.01	J/mol×K	1070.50	Joback Method
cpg	1002.84	J/mol×K	1111.48	Joback Method
cpg	1011.19	J/mol×K	1152.46	Joback Method
cpg	1018.12	J/mol×K	1193.45	Joback Method
cpg	1023.68	J/mol×K	1234.43	Joback Method
cpg	1027.95	J/mol×K	1275.41	Joback Method
cpg	1030.98	J/mol×K	1316.39	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=U382525&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