Phthalic acid, decyl 4-nitrobenzyl ester

Inchi: InChI=1S/C25H31NO6/c1-2-3-4-5-6-7-8-11-18-31-24(27)22-12-9-10-13-23(22)25(28)32-
InchiKey: PLEKPRPWVXSJGH-UHFFFAOYSA-N
Formula: C25H31NO6
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 441.52

Physical Properties

Property code	Value	Unit	Source
gf	-67.11	kJ/mol	Joback Method
hf	-609.57	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	112.02	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	6.249		Crippen Method
mcvol	347.890	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	3960.00		NIST Webbook
rinpol	3960.00		NIST Webbook
tb	1139.14	K	Joback Method
tc	1394.65	K	Joback Method
tf	737.32	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.56	J/mol×K	1139.14	Joback Method
cpg	1181.35	J/mol×K	1181.72	Joback Method
cpg	1189.52	J/mol×K	1224.31	Joback Method
cpg	1196.16	J/mol×K	1266.89	Joback Method
cpg	1201.34	J/mol×K	1309.48	Joback Method
cpg	1205.15	J/mol×K	1352.06	Joback Method
cpg	1207.68	J/mol×K	1394.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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