Phthalic acid, decyl 4-methyl-3-nitrobenzyl ester

Inchi: InChI=1S/C26H33NO6/c1-3-4-5-6-7-8-9-12-17-32-25(28)22-13-10-11-14-23(22)26(29)33

InchiKey: OGQKDSNAWBKEGT-UHFFFAOYSA-N

Formula: C26H33NO6

SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(C)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 455.54

Physical Properties

Property code	Value	Unit	Source
gf	-68.32	kJ/mol	Joback Method
hf	-641.68	kJ/mol	Joback Method
hfus	66.95	kJ/mol	Joback Method
hvap	114.91	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	6.558		Crippen Method
mcvol	361.980	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	3794.00		NIST Webbook
rinpol	3794.00		NIST Webbook
tb	1167.00	K	Joback Method
tc	1429.24	K	Joback Method
tf	761.11	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1229.55	J/mol×K	1167.00	Joback Method
cpg	1238.93	J/mol×K	1210.71	Joback Method
cpg	1246.54	J/mol×K	1254.41	Joback Method
cpg	1252.46	J/mol×K	1298.12	Joback Method
cpg	1256.76	J/mol×K	1341.82	Joback Method
cpg	1259.53	J/mol×K	1385.53	Joback Method
cpg	1260.86	J/mol×K	1429.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382588&Units=SI

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