p-Nitrophenyl p-decyloxybenzoate

Inchi: InChI=1S/C23H29NO5/c1-2-3-4-5-6-7-8-9-18-28-21-14-10-19(11-15-21)23(25)29-22-16-
InchiKey: SYQHCBATGVPGPV-UHFFFAOYSA-N
Formula: C23H29NO5
SMILES: CCCCCCCCCCOc1ccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 399.48
CAS: 63635-84-7

Physical Properties

Property code	Value	Unit	Source
gf	44.97	kJ/mol	Joback Method
hf	-455.71	kJ/mol	Joback Method
hfus	57.97	kJ/mol	Joback Method
hvap	100.83	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.333		Crippen Method
mcvol	318.140	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
tb	1039.51	K	Joback Method
tc	1278.32	K	Joback Method
tf	664.85	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.68	J/mol×K	1039.51	Joback Method
cpg	1060.91	J/mol×K	1079.31	Joback Method
cpg	1071.68	J/mol×K	1119.11	Joback Method
cpg	1081.06	J/mol×K	1158.92	Joback Method
cpg	1089.11	J/mol×K	1198.72	Joback Method
cpg	1095.89	J/mol×K	1238.52	Joback Method
cpg	1101.46	J/mol×K	1278.32	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=C63635847&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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