Terephthalic acid, hexyl 4-nitro-3-methylbenzyl ester

Inchi: InChI=1S/C22H25NO6/c1-3-4-5-6-13-28-21(24)18-8-10-19(11-9-18)22(25)29-15-17-7-12

InchiKey: AAWPCUKEQQOBMC-UHFFFAOYSA-N

Formula: C22H25NO6

SMILES: CCCCCCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])c(C)c2)cc1

Mol. weight [g/mol]: 399.44

Physical Properties

Property code	Value	Unit	Source
gf	-102.00	kJ/mol	Joback Method
hf	-559.12	kJ/mol	Joback Method
hfus	56.59	kJ/mol	Joback Method
hvap	106.01	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	4.997		Crippen Method
mcvol	305.620	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	1075.48	K	Joback Method
tc	1322.27	K	Joback Method
tf	716.03	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.18	J/mol×K	1075.48	Joback Method
cpg	1000.77	J/mol×K	1116.61	Joback Method
cpg	1008.81	J/mol×K	1157.74	Joback Method
cpg	1015.37	J/mol×K	1198.87	Joback Method
cpg	1020.49	J/mol×K	1240.00	Joback Method
cpg	1024.22	J/mol×K	1281.14	Joback Method
cpg	1026.61	J/mol×K	1322.27	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=U416103&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