Isophthalic acid, heptyl 4-nitrophenyl ester

Inchi: InChI=1S/C21H23NO6/c1-2-3-4-5-6-14-27-20(23)16-8-7-9-17(15-16)21(24)28-19-12-10-
InchiKey: URCIIXVSRBXXES-UHFFFAOYSA-N
Formula: C21H23NO6
SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)c1
Mol. weight [g/mol]: 385.41

Physical Properties

Property code	Value	Unit	Source
gf	-100.79	kJ/mol	Joback Method
hf	-527.01	kJ/mol	Joback Method
hfus	54.38	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	4.941		Crippen Method
mcvol	291.530	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1047.62	K	Joback Method
tc	1292.43	K	Joback Method
tf	692.24	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.26	J/mol×K	1047.62	Joback Method
cpg	944.10	J/mol×K	1088.42	Joback Method
cpg	952.50	J/mol×K	1129.22	Joback Method
cpg	959.49	J/mol×K	1170.03	Joback Method
cpg	965.15	J/mol×K	1210.83	Joback Method
cpg	969.52	J/mol×K	1251.63	Joback Method
cpg	972.66	J/mol×K	1292.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344684&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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