Terephthalic acid, 2-nitrobenzyl pentyl ester

Inchi: InChI=1S/C20H21NO6/c1-2-3-6-13-26-19(22)15-9-11-16(12-10-15)20(23)27-14-17-7-4-5
InchiKey: BDYOUEYLEHVQTA-UHFFFAOYSA-N
Formula: C20H21NO6
SMILES: CCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2[N+](=O)[O-])cc1
Mol. weight [g/mol]: 371.38

Physical Properties

Property code	Value	Unit	Source
gf	-109.21	kJ/mol	Joback Method
hf	-506.37	kJ/mol	Joback Method
hfus	51.79	kJ/mol	Joback Method
hvap	100.89	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.299		Crippen Method
mcvol	277.440	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	1024.74	K	Joback Method
tc	1269.43	K	Joback Method
tf	680.97	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.97	J/mol×K	1024.74	Joback Method
cpg	885.81	J/mol×K	1065.52	Joback Method
cpg	894.23	J/mol×K	1106.30	Joback Method
cpg	901.28	J/mol×K	1147.09	Joback Method
cpg	907.01	J/mol×K	1187.87	Joback Method
cpg	911.45	J/mol×K	1228.65	Joback Method
cpg	914.67	J/mol×K	1269.43	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=U416117&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