Terephthalic acid, isobutyl 4-nitrobenzyl ester

Inchi: InChI=1S/C19H19NO6/c1-13(2)11-25-18(21)15-5-7-16(8-6-15)19(22)26-12-14-3-9-17(10
InchiKey: VRGLXXGRRRHWQM-UHFFFAOYSA-N
Formula: C19H19NO6
SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 357.36

Physical Properties

Property code	Value	Unit	Source
gf	-120.07	kJ/mol	Joback Method
hf	-491.01	kJ/mol	Joback Method
hfus	45.68	kJ/mol	Joback Method
hvap	98.28	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	3.765		Crippen Method
mcvol	263.350	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		NIST Webbook
tb	1001.42	K	Joback Method
tc	1249.54	K	Joback Method
tf	654.70	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.60	J/mol×K	1001.42	Joback Method
cpg	828.45	J/mol×K	1042.77	Joback Method
cpg	836.86	J/mol×K	1084.13	Joback Method
cpg	843.86	J/mol×K	1125.48	Joback Method
cpg	849.51	J/mol×K	1166.83	Joback Method
cpg	853.85	J/mol×K	1208.19	Joback Method
cpg	856.92	J/mol×K	1249.54	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=U416161&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

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