Terephthalic acid, ethyl 4-nitrobenzyl ester

Inchi: InChI=1S/C17H15NO6/c1-2-23-16(19)13-5-7-14(8-6-13)17(20)24-11-12-3-9-15(10-4-12)
InchiKey: HUISEFDBGNNORG-UHFFFAOYSA-N
Formula: C17H15NO6
SMILES: CCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 329.30

Physical Properties

Property code	Value	Unit	Source
gf	-134.47	kJ/mol	Joback Method
hf	-444.45	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	94.22	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	3.128		Crippen Method
mcvol	235.170	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	956.10	K	Joback Method
tc	1205.77	K	Joback Method
tf	647.16	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.28	J/mol×K	956.10	Joback Method
cpg	714.02	J/mol×K	997.71	Joback Method
cpg	722.38	J/mol×K	1039.32	Joback Method
cpg	729.42	J/mol×K	1080.94	Joback Method
cpg	735.16	J/mol×K	1122.55	Joback Method
cpg	739.63	J/mol×K	1164.16	Joback Method
cpg	742.88	J/mol×K	1205.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416159&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