Terephthalic acid, ethyl 2-(3-nitrophenyl)ethyl ester

Inchi: InChI=1S/C18H17NO6/c1-2-24-17(20)14-6-8-15(9-7-14)18(21)25-11-10-13-4-3-5-16(12-
InchiKey: UTICNDAXLMGVKD-UHFFFAOYSA-N
Formula: C18H17NO6
SMILES: CCOC(=O)c1ccc(C(=O)OCCc2cccc([N+](=O)[O-])c2)cc1
Mol. weight [g/mol]: 343.33

Physical Properties

Property code	Value	Unit	Source
gf	-126.05	kJ/mol	Joback Method
hf	-465.09	kJ/mol	Joback Method
hfus	46.61	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.171		Crippen Method
mcvol	249.260	ml/mol	McGowan Method
pc	2047.46	kPa	Joback Method
rinpol	2994.00		NIST Webbook
rinpol	2994.00		NIST Webbook
tb	978.98	K	Joback Method
tc	1226.15	K	Joback Method
tf	658.43	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.93	J/mol×K	978.98	Joback Method
cpg	770.73	J/mol×K	1020.17	Joback Method
cpg	779.14	J/mol×K	1061.37	Joback Method
cpg	786.21	J/mol×K	1102.56	Joback Method
cpg	791.98	J/mol×K	1143.76	Joback Method
cpg	796.49	J/mol×K	1184.95	Joback Method
cpg	799.77	J/mol×K	1226.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416104&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