Terephthalic acid, ethyl 4-nitro-3-methylbenzyl ester

Inchi: InChI=1S/C18H17NO6/c1-3-24-17(20)14-5-7-15(8-6-14)18(21)25-11-13-4-9-16(19(22)23
InchiKey: ZXLKLPJAXJEZLH-UHFFFAOYSA-N
Formula: C18H17NO6
SMILES: CCOC(=O)c1ccc(C(=O)OCc2ccc([N+](=O)[O-])c(C)c2)cc1
Mol. weight [g/mol]: 343.33

Physical Properties

Property code	Value	Unit	Source
gf	-135.68	kJ/mol	Joback Method
hf	-476.56	kJ/mol	Joback Method
hfus	46.23	kJ/mol	Joback Method
hvap	97.10	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	3.437		Crippen Method
mcvol	249.260	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	983.96	K	Joback Method
tc	1231.84	K	Joback Method
tf	670.95	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.15	J/mol×K	983.96	Joback Method
cpg	768.79	J/mol×K	1025.27	Joback Method
cpg	777.02	J/mol×K	1066.59	Joback Method
cpg	783.86	J/mol×K	1107.90	Joback Method
cpg	789.34	J/mol×K	1149.22	Joback Method
cpg	793.49	J/mol×K	1190.53	Joback Method
cpg	796.34	J/mol×K	1231.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416098&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