Benzoic acid, (2-methyl-3-nitrophenyl)methyl ester

Inchi: InChI=1S/C15H13NO4/c1-11-13(8-5-9-14(11)16(18)19)10-20-15(17)12-6-3-2-4-7-12/h2-9

InchiKey: PHKGZQABUFXZDA-UHFFFAOYSA-N

Formula: C15H13NO4

SMILES: Cc1c(COC(=O)c2ccccc2)cccc1[N+](=O)[O-]

Mol. weight [g/mol]: 271.27

Physical Properties

Property code	Value	Unit	Source
gf	82.61	kJ/mol	Joback Method
hf	-158.37	kJ/mol	Joback Method
hfus	36.06	kJ/mol	Joback Method
hvap	80.61	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.260		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	834.05	K	Joback Method
tc	1090.64	K	Joback Method
tf	552.46	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.71	J/mol×K	834.05	Joback Method
cpg	575.05	J/mol×K	876.82	Joback Method
cpg	586.14	J/mol×K	919.58	Joback Method
cpg	596.04	J/mol×K	962.35	Joback Method
cpg	604.80	J/mol×K	1005.11	Joback Method
cpg	612.49	J/mol×K	1047.88	Joback Method
cpg	619.16	J/mol×K	1090.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367950&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

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