4-Butylbenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C17H17NO4/c1-2-3-4-13-5-7-14(8-6-13)17(19)22-16-11-9-15(10-12-16)18(20)
InchiKey: VVCMTMMBNVKTTG-UHFFFAOYSA-N
Formula: C17H17NO4
SMILES: CCCCc1ccc(C(=O)Oc2ccc([N+](=O)[O-])cc2)cc1
Mol. weight [g/mol]: 299.32

Physical Properties

Property code	Value	Unit	Source
gf	99.45	kJ/mol	Joback Method
hf	-199.65	kJ/mol	Joback Method
hfus	41.24	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	4.157		Crippen Method
mcvol	227.730	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2526.00		NIST Webbook
rinpol	2526.00		NIST Webbook
tb	879.81	K	Joback Method
tc	1127.16	K	Joback Method
tf	575.00	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.21	J/mol×K	879.81	Joback Method
cpg	685.98	J/mol×K	921.04	Joback Method
cpg	697.49	J/mol×K	962.26	Joback Method
cpg	707.82	J/mol×K	1003.49	Joback Method
cpg	717.02	J/mol×K	1044.71	Joback Method
cpg	725.16	J/mol×K	1085.94	Joback Method
cpg	732.29	J/mol×K	1127.16	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=U307509&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