Benzoic acid, 4-nitro, 1-phenylethyl ester

Inchi: InChI=1S/C15H13NO4/c1-11(12-5-3-2-4-6-12)20-15(17)13-7-9-14(10-8-13)16(18)19/h2-1
InchiKey: HVSDVQCMFAIRJJ-UHFFFAOYSA-N
Formula: C15H13NO4
SMILES: CC(OC(=O)c1ccc([N+](=O)[O-])cc1)c1ccccc1
Mol. weight [g/mol]: 271.27

Physical Properties

Property code	Value	Unit	Source
gf	89.80	kJ/mol	Joback Method
hf	-152.18	kJ/mol	Joback Method
hfus	32.92	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.513		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2123.00		NIST Webbook
tb	828.63	K	Joback Method
tc	1089.25	K	Joback Method
tf	524.94	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.92	J/mol×K	828.63	Joback Method
cpg	577.56	J/mol×K	872.07	Joback Method

cpg	588.88	J/mol×K	915.50	Joback Method
cpg	598.95	J/mol×K	958.94	Joback Method
cpg	607.85	J/mol×K	1002.38	Joback Method
cpg	615.64	J/mol×K	1045.82	Joback Method
cpg	622.41	J/mol×K	1089.25	Joback Method

Sources

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=R35111&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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