Benzoic acid, 2-(4-nitrophenoxy)ethyl ester

Inchi: InChI=1S/C15H13NO5/c17-15(12-4-2-1-3-5-12)21-11-10-20-14-8-6-13(7-9-14)16(18)19/h
InchiKey: RQYJKKRYSQSUIT-UHFFFAOYSA-N
Formula: C15H13NO5
SMILES: O=C(OCCOc1ccc([N+](=O)[O-])cc1)c1ccccc1
Mol. weight [g/mol]: 287.27

Physical Properties

Property code	Value	Unit	Source
gf	-12.76	kJ/mol	Joback Method
hf	-279.12	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.831		Crippen Method
mcvol	205.420	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	851.49	K	Joback Method
tc	1103.59	K	Joback Method
tf	562.17	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.35	J/mol×K	851.49	Joback Method
cpg	601.17	J/mol×K	893.51	Joback Method
cpg	611.68	J/mol×K	935.52	Joback Method
cpg	620.92	J/mol×K	977.54	Joback Method
cpg	628.93	J/mol×K	1019.56	Joback Method
cpg	635.75	J/mol×K	1061.57	Joback Method
cpg	641.43	J/mol×K	1103.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368927&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