4-Nitrobenzoic acid, 2-phenylethyl ester

Other names: Benzoic acid, 4-nitro, 2-phenylethyl ester
Inchi: InChI=1S/C15H13NO4/c17-15(13-6-8-14(9-7-13)16(18)19)20-11-10-12-4-2-1-3-5-12/h1-9
InchiKey: WFYVRFBHTYEHJV-UHFFFAOYSA-N
Formula: C15H13NO4
SMILES: O=C(OCCc1ccccc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 271.27
CAS: 57455-00-2

Physical Properties

Property code	Value	Unit	Source
gf	92.24	kJ/mol	Joback Method
hf	-146.90	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	79.95	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	2.994		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	2169.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2201.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	829.07	K	Joback Method
tc	1084.98	K	Joback Method
tf	539.94	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.32	J/mol×K	829.07	Joback Method
cpg	576.75	J/mol×K	871.72	Joback Method
cpg	587.93	J/mol×K	914.37	Joback Method
cpg	597.92	J/mol×K	957.02	Joback Method
cpg	606.79	J/mol×K	999.67	Joback Method
cpg	614.61	J/mol×K	1042.33	Joback Method
cpg	621.45	J/mol×K	1084.98	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=C57455002&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

Latest version available from:
https://www.chemeo.com/cid/47-138-7/4-Nitrobenzoic-acid-2-phenylethyl-ester.pdf
Generated by Cheméo on 2024-04-20 11:45:24.78693536 +0000 UTC m=+15902773.707512682.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.