Benzoic acid, 4-nitro-, phenylmethyl ester

Other names:	Benzoic acid, p-nitro-, benzyl ester
	Benzyl p-nitrobenzoate
	Benzyl 4-nitrobenzoate
	4-Nitrobenzoic acid, benzyl ester
	Benzoic acid, 4-nitro, benzyl ester
Inchi:	InChI=1S/C14H11NO4/c16-14(19-10-11-4-2-1-3-5-11)12-6-8-13(9-7-12)15(17)18/h1-9H,
InchiKey:	XCQFGJYVKKCUFX-UHFFFAOYSA-N
Formula:	C14H11NO4
SMILES:	O=C(OCc1ccccc1)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	257.24
CAS:	14786-27-7

Physical Properties

Property code	Value	Unit	Source
gf	83.82	kJ/mol	Joback Method
hf	-126.26	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	77.72	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	2.952		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2071.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2097.00		NIST Webbook
rinpol	2106.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	806.19	K	Joback Method
tc	1067.65	K	Joback Method
tf	528.67	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.55	J/mol×K	806.19	Joback Method
cpg	522.67	J/mol×K	849.77	Joback Method
cpg	533.54	J/mol×K	893.34	Joback Method
cpg	543.22	J/mol×K	936.92	Joback Method
cpg	551.78	J/mol×K	980.50	Joback Method
cpg	559.28	J/mol×K	1024.08	Joback Method
cpg	565.80	J/mol×K	1067.65	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=C14786277&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