Benzoic acid, (4-methoxy-3-nitrophenyl)methyl ester

Inchi: InChI=1S/C15H13NO5/c1-20-14-8-7-11(9-13(14)16(18)19)10-21-15(17)12-5-3-2-4-6-12/h
InchiKey: FNYWSBFCTMNWGN-UHFFFAOYSA-N
Formula: C15H13NO5
SMILES: COc1ccc(COC(=O)c2ccccc2)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 287.27

Physical Properties

Property code	Value	Unit	Source
gf	-22.39	kJ/mol	Joback Method
hf	-290.59	kJ/mol	Joback Method
hfus	37.25	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	2.960		Crippen Method
mcvol	205.420	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	2553.00		NIST Webbook
tb	856.47	K	Joback Method
tc	1109.25	K	Joback Method
tf	574.69	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.71	J/mol×K	856.47	Joback Method
cpg	599.43	J/mol×K	898.60	Joback Method
cpg	609.84	J/mol×K	940.73	Joback Method
cpg	618.96	J/mol×K	982.86	Joback Method
cpg	626.83	J/mol×K	1024.99	Joback Method
cpg	633.48	J/mol×K	1067.12	Joback Method
cpg	638.94	J/mol×K	1109.25	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=U368923&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/38-643-6/Benzoic-acid-4-methoxy-3-nitrophenyl-methyl-ester.pdf
Generated by Cheméo on 2024-04-27 05:48:56.900463328 +0000 UTC m=+16486185.821040644.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.