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

Inchi: InChI=1S/C9H9NO5/c1-14-9-3-2-7(5-15-6-11)4-8(9)10(12)13/h2-4,6H,5H2,1H3
InchiKey: VFCJZZYJXYIJQS-UHFFFAOYSA-N
Formula: C9H9NO5
SMILES: COc1ccc(COC=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 211.17

Physical Properties

Property code	Value	Unit	Source
gf	-155.92	kJ/mol	Joback Method
hf	-376.28	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.276		Crippen Method
mcvol	144.640	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1809.00		NIST Webbook
tb	687.30	K	Joback Method
tc	921.78	K	Joback Method
tf	472.72	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.54	J/mol×K	687.30	Joback Method
cpg	379.40	J/mol×K	726.38	Joback Method
cpg	389.47	J/mol×K	765.46	Joback Method
cpg	398.75	J/mol×K	804.54	Joback Method
cpg	407.24	J/mol×K	843.62	Joback Method
cpg	414.92	J/mol×K	882.70	Joback Method
cpg	421.78	J/mol×K	921.78	Joback Method

Sources

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=U368921&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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