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

Inchi: InChI=1S/C9H9NO4/c1-7-2-3-8(5-14-6-11)4-9(7)10(12)13/h2-4,6H,5H2,1H3
InchiKey: ORFBBOBPAWUFAS-UHFFFAOYSA-N
Formula: C9H9NO4
SMILES: Cc1ccc(COC=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 195.17

Physical Properties

Property code	Value	Unit	Source
gf	-50.92	kJ/mol	Joback Method
hf	-244.06	kJ/mol	Joback Method
hfus	27.17	kJ/mol	Joback Method
hvap	64.95	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.576		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
rinpol	1610.00		NIST Webbook
tb	664.88	K	Joback Method
tc	902.91	K	Joback Method
tf	450.49	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.52	J/mol×K	664.88	Joback Method
cpg	356.53	J/mol×K	704.55	Joback Method
cpg	366.74	J/mol×K	744.22	Joback Method
cpg	376.18	J/mol×K	783.89	Joback Method
cpg	384.86	J/mol×K	823.56	Joback Method
cpg	392.79	J/mol×K	863.24	Joback Method
cpg	399.98	J/mol×K	902.91	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=U368226&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

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