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

Inchi: InChI=1S/C10H11NO5/c1-7(12)16-6-8-3-4-10(15-2)9(5-8)11(13)14/h3-5H,6H2,1-2H3
InchiKey: GQZJPLTVIHEURG-UHFFFAOYSA-N
Formula: C10H11NO5
SMILES: COc1ccc(COC(C)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 225.20

Physical Properties

Property code	Value	Unit	Source
gf	-176.90	kJ/mol	Joback Method
hf	-423.92	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	69.61	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.666		Crippen Method
mcvol	158.730	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1878.00		NIST Webbook
tb	715.39	K	Joback Method
tc	950.05	K	Joback Method
tf	491.92	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.63	J/mol×K	715.39	Joback Method
cpg	429.41	J/mol×K	754.50	Joback Method
cpg	440.30	J/mol×K	793.61	Joback Method
cpg	450.30	J/mol×K	832.72	Joback Method
cpg	459.40	J/mol×K	871.83	Joback Method
cpg	467.61	J/mol×K	910.94	Joback Method
cpg	474.90	J/mol×K	950.05	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=U368922&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