2-Methylpropionic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C10H11NO4/c1-7(2)10(12)15-9-5-3-8(4-6-9)11(13)14/h3-7H,1-2H3
InchiKey: AIKAOGTVMFOQKJ-UHFFFAOYSA-N
Formula: C10H11NO4
SMILES: CC(C)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 209.20

Physical Properties

Property code	Value	Unit	Source
gf	-64.71	kJ/mol	Joback Method
hf	-285.51	kJ/mol	Joback Method
hfus	25.93	kJ/mol	Joback Method
hvap	66.15	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.156		Crippen Method
mcvol	152.860	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1576.00		NIST Webbook
rinpol	1576.00		NIST Webbook
tb	687.55	K	Joback Method
tc	929.72	K	Joback Method
tf	442.17	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.71	J/mol×K	687.55	Joback Method
cpg	408.14	J/mol×K	727.91	Joback Method
cpg	419.60	J/mol×K	768.27	Joback Method
cpg	430.12	J/mol×K	808.64	Joback Method
cpg	439.73	J/mol×K	849.00	Joback Method
cpg	448.44	J/mol×K	889.36	Joback Method
cpg	456.29	J/mol×K	929.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308020&Units=SI
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

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