3-Methylbut-2-enoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C11H11NO4/c1-8(2)7-11(13)16-10-5-3-9(4-6-10)12(14)15/h3-7H,1-2H3
InchiKey: UWHFXNUVALKMIU-UHFFFAOYSA-N
Formula: C11H11NO4
SMILES: CC(C)=CC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 221.21

Physical Properties

Property code	Value	Unit	Source
gf	17.82	kJ/mol	Joback Method
hf	-193.44	kJ/mol	Joback Method
hfus	30.94	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.466		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
rinpol	1778.00		NIST Webbook
tb	714.91	K	Joback Method
tc	960.88	K	Joback Method
tf	449.40	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.40	J/mol×K	714.91	Joback Method
cpg	433.64	J/mol×K	755.91	Joback Method
cpg	444.90	J/mol×K	796.90	Joback Method
cpg	455.25	J/mol×K	837.90	Joback Method
cpg	464.73	J/mol×K	878.89	Joback Method
cpg	473.39	J/mol×K	919.89	Joback Method
cpg	481.29	J/mol×K	960.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307598&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