Acetoxyacetic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C10H9NO6/c1-7(12)16-6-10(13)17-9-4-2-8(3-5-9)11(14)15/h2-5H,6H2,1H3
InchiKey: XGFYUGQGRUDVPI-UHFFFAOYSA-N
Formula: C10H9NO6
SMILES: CC(=O)OCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 239.18

Physical Properties

Property code	Value	Unit	Source
gf	-296.19	kJ/mol	Joback Method
hf	-525.03	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.063		Crippen Method
mcvol	160.300	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1772.00		NIST Webbook
tb	764.28	K	Joback Method
tc	1003.42	K	Joback Method
tf	529.33	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.18	J/mol×K	764.28	Joback Method
cpg	438.44	J/mol×K	804.14	Joback Method
cpg	447.75	J/mol×K	843.99	Joback Method
cpg	456.09	J/mol×K	883.85	Joback Method
cpg	463.48	J/mol×K	923.71	Joback Method
cpg	469.90	J/mol×K	963.56	Joback Method
cpg	475.37	J/mol×K	1003.42	Joback Method

Sources

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=U307545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/29-603-0/Acetoxyacetic-acid-4-nitrophenyl-ester.pdf
Generated by Cheméo on 2024-04-19 02:27:34.310305127 +0000 UTC m=+15782903.230882443.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.