

P-nitro cinnamic acid, methyl ester

Inchi:	InChI=1S/C10H9NO4/c1-15-10(12)7-4-8-2-5-9(6-3-8)11(13)14/h2-7H,1H3/b7-4+
InchiKey:	NVXKMHUNXMXXDM-QPJXVBHSA-N
Formula:	C10H9NO4
SMILES:	<chem>COC(=O)C=Cc1ccc([N+](=O)[O-])cc1</chem>
Mol. weight [g/mol]:	207.18
CAS:	1608-36-2

Physical Properties

Property code	Value	Unit	Source
gf	17.95	kJ/mol	Joback Method
hf	-163.01	kJ/mol	Joback Method
hfus	29.66	kJ/mol	Joback Method
hvap	66.50	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.781		Crippen Method
mcvol	148.560	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	692.15	K	Joback Method
tc	939.29	K	Joback Method
tf	452.09	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.69	J/molxK	692.15	Joback Method
cpg	383.11	J/molxK	733.34	Joback Method
cpg	393.60	J/molxK	774.53	Joback Method
cpg	403.23	J/molxK	815.72	Joback Method
cpg	412.03	J/molxK	856.91	Joback Method
cpg	420.05	J/molxK	898.10	Joback Method
cpg	427.33	J/molxK	939.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1608362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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