P-anisamide, 3-nitro-

Other names: 3-nitro-p-anisamide
Inchi: InChI=1S/C8H8N2O4/c1-14-7-3-2-5(8(9)11)4-6(7)10(12)13/h2-4H,1H3,(H2,9,11)
InchiKey: PCQFJXUTKOUTRW-UHFFFAOYSA-N
Formula: C8H8N2O4
SMILES: COc1ccc(C(N)=O)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 196.16
CAS: 10397-58-7

Physical Properties

Property code	Value	Unit	Source
gf	-22.29	kJ/mol	Joback Method
hf	-216.63	kJ/mol	Joback Method
hfus	29.08	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	0.702		Crippen Method
mcvol	134.660	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	719.74	K	Joback Method
tc	973.32	K	Joback Method
tf	530.41	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.10	J/mol×K	719.74	Joback Method
cpg	357.01	J/mol×K	762.00	Joback Method
cpg	366.06	J/mol×K	804.27	Joback Method
cpg	374.27	J/mol×K	846.53	Joback Method
cpg	381.65	J/mol×K	888.80	Joback Method
cpg	388.20	J/mol×K	931.06	Joback Method
cpg	393.95	J/mol×K	973.32	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=C10397587&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume