o-Nitrocinnamide

Other names: o-Nitrobenzylidene acetamide
Inchi: InChI=1S/C9H8N2O3/c10-9(12)6-5-7-3-1-2-4-8(7)11(13)14/h1-6H,(H2,10,12)/b6-5+
InchiKey: RASLWNGTMHFPIQ-AATRIKPKSA-N
Formula: C9H8N2O3
SMILES: NC(=O)C=Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 192.17
CAS: 2001-33-4

Physical Properties

Property code	Value	Unit	Source
chs	-4539.89	kJ/mol	NIST Webbook
gf	180.98	kJ/mol	Joback Method
hf	23.64	kJ/mol	Joback Method
hfs	-144.70	kJ/mol	NIST Webbook
hfus	31.08	kJ/mol	Joback Method
hvap	72.50	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.093		Crippen Method
mcvol	138.580	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	719.38	K	Joback Method
tc	981.27	K	Joback Method
tf	501.85	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.20	J/mol×K	719.38	Joback Method
cpg	361.34	J/mol×K	763.03	Joback Method
cpg	370.57	J/mol×K	806.68	Joback Method
cpg	378.99	J/mol×K	850.32	Joback Method
cpg	386.66	J/mol×K	893.97	Joback Method
cpg	393.67	J/mol×K	937.62	Joback Method

cpg	400.11	J/mol×K	981.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2001334&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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