

trans-2-Nitrocinnamic acid

Other names:	2-Nitrocinnamic acid o-Nitrocinnamic acid 2-Propenoic acid, 3-(2-nitrophenyl)- Cinnamic acid, o-nitro-
Inchi:	InChI=1S/C9H7NO4/c11-9(12)6-5-7-3-1-2-4-8(7)10(13)14/h1-6H,(H,11,12)/b6-5+
InchiKey:	BBQDLDVSEDAYAA-AATRIKPKSA-N
Formula:	C9H7NO4
SMILES:	O=C(O)C=Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	193.16
CAS:	612-41-9

Physical Properties

Property code	Value	Unit	Source
chs	-4162.00	kJ/mol	NIST Webbook
chs	-4179.93	kJ/mol	NIST Webbook
gf	-22.29	kJ/mol	Joback Method
hf	-162.38	kJ/mol	Joback Method
hfs	-379.90	kJ/mol	NIST Webbook
hfus	29.97	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.693		Crippen Method
mcvol	134.470	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
tb	739.03	K	Joback Method
tc	973.12	K	Joback Method
tf	479.41	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.68	J/mol×K	739.03	Joback Method
cpg	349.01	J/mol×K	778.04	Joback Method

cpg	356.67	J/mol×K	817.06	Joback Method
cpg	363.73	J/mol×K	856.07	Joback Method
cpg	370.23	J/mol×K	895.09	Joback Method
cpg	376.23	J/mol×K	934.10	Joback Method
cpg	381.80	J/mol×K	973.12	Joback Method
cps	240.60	J/mol×K	323.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C612419&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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

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