m-Aminocinnamic acid

Inchi: InChI=1S/C9H9NO2/c10-8-3-1-2-7(6-8)4-5-9(11)12/h1-6H,10H2,(H,11,12)/b5-4+
InchiKey: JNXMJSYJCFTLJB-SNAWJCMRSA-N
Formula: C9H9NO2
SMILES: Nc1cccc(C=CC(=O)O)c1
Mol. weight [g/mol]: 163.17
CAS: 1664-56-8

Physical Properties

Property code	Value	Unit	Source
gf	8.61	kJ/mol	Joback Method
hf	-117.83	kJ/mol	Joback Method
hfus	23.80	kJ/mol	Joback Method
hvap	72.59	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.367		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	4432.62	kPa	Joback Method
tb	659.72	K	Joback Method
tc	879.89	K	Joback Method
tf	419.06	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.42	J/mol×K	659.72	Joback Method
cpg	319.65	J/mol×K	696.41	Joback Method
cpg	328.23	J/mol×K	733.11	Joback Method
cpg	336.20	J/mol×K	769.80	Joback Method
cpg	343.60	J/mol×K	806.50	Joback Method
cpg	350.48	J/mol×K	843.19	Joback Method
cpg	356.90	J/mol×K	879.89	Joback Method
cps	227.60	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=C1664568&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

cpg:	Ideal gas heat capacity
cps:	Solid phase 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