«alpha»-Cyano-3-hydroxycinnamic acid

Other names: 2-Propenoic acid, 2-cyano-3-(3-hydroxyphenyl)-
alpha-cyano-m-hydroxycinnamic acid
Inchi: InChI=1S/C10H7NO3/c11-6-8(10(13)14)4-7-2-1-3-9(12)5-7/h1-5,12H,(H,13,14)/b8-4+
InchiKey: HPLNTJVXWMJLNJ-XBXARRHUSA-N
Formula: C10H7NO3
SMILES: N#CC(=Cc1cccc(O)c1)C(=O)O
Mol. weight [g/mol]: 189.17
CAS: 54673-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-69.78	kJ/mol	Joback Method
hf	-183.01	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.384		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	787.67	K	Joback Method
tc	1019.81	K	Joback Method
tf	497.30	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.63	J/mol×K	787.67	Joback Method
cpg	362.77	J/mol×K	826.36	Joback Method
cpg	369.59	J/mol×K	865.05	Joback Method
cpg	376.20	J/mol×K	903.74	Joback Method
cpg	382.72	J/mol×K	942.43	Joback Method
cpg	389.23	J/mol×K	981.12	Joback Method
cpg	395.87	J/mol×K	1019.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54673073&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
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