3-Buten-2-one, 4-hydroxy-4-(phenylamino)-

Inchi: InChI=1S/C10H11NO2/c1-8(12)7-10(13)11-9-5-3-2-4-6-9/h2-7,11,13H,1H3/b10-7-
InchiKey: IGKMBTGLQPCPNS-YFHOEESVSA-N
Formula: C10H11NO2
SMILES: CC(=O)C=C(O)Nc1ccccc1
Mol. weight [g/mol]: 177.20
CAS: 114113-11-0

Physical Properties

Property code	Value	Unit	Source
gf	41.05	kJ/mol	Joback Method
hf	-117.11	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	70.03	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.087		Crippen Method
mcvol	141.120	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	655.14	K	Joback Method
tc	866.76	K	Joback Method
tf	373.25	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.53	J/mol×K	655.14	Joback Method
cpg	363.15	J/mol×K	690.41	Joback Method
cpg	373.04	J/mol×K	725.68	Joback Method
cpg	382.24	J/mol×K	760.95	Joback Method
cpg	390.81	J/mol×K	796.22	Joback Method
cpg	398.79	J/mol×K	831.49	Joback Method
cpg	406.24	J/mol×K	866.76	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=C114113110&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