3-Buten-2-one, 4-[(4-chlorophenyl)amino]-4-hydroxy-

Inchi: InChI=1S/C10H10ClNO2/c1-7(13)6-10(14)12-9-4-2-8(11)3-5-9/h2-6,12,14H,1H3/b10-6-

InchiKey: FNZYEPGRAPXOIZ-POHAHGRESA-N

Formula: C10H10ClNO2

SMILES: CC(=O)C=C(O)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 211.65

CAS: 114113-14-3

Physical Properties

Property code	Value	Unit	Source
gf	19.49	kJ/mol	Joback Method
hf	-144.32	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.740		Crippen Method
mcvol	153.360	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	697.55	K	Joback Method
tc	913.30	K	Joback Method
tf	415.69	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.94	J/mol×K	697.55	Joback Method
cpg	382.49	J/mol×K	733.51	Joback Method
cpg	391.38	J/mol×K	769.47	Joback Method
cpg	399.64	J/mol×K	805.43	Joback Method
cpg	407.32	J/mol×K	841.38	Joback Method
cpg	414.49	J/mol×K	877.34	Joback Method
cpg	421.18	J/mol×K	913.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114113143&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

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