1-(5'-Chloro-2'-methylaminobenzoyl)-cyclohex-1-e

Other names: 1-Cyclohexenyl 5-chloro-2-methylaminophenyl ketone
Inchi: InChI=1S/C14H16ClNO/c1-16-13-8-7-11(15)9-12(13)14(17)10-5-3-2-4-6-10/h5,7-9,16H,2
InchiKey: CZSVMGRCLAQSME-UHFFFAOYSA-N
Formula: C14H16ClNO
SMILES: CNc1ccc(Cl)cc1C(=O)C1=CCCCC1
Mol. weight [g/mol]: 249.74
CAS: 97994-57-5

Physical Properties

Property code	Value	Unit	Source
gf	161.18	kJ/mol	Joback Method
hf	-72.58	kJ/mol	Joback Method
hfus	27.77	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.065		Crippen Method
mcvol	192.990	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2247.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2232.00		NIST Webbook
tb	726.19	K	Joback Method
tc	969.55	K	Joback Method
tf	456.41	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.84	J/mol×K	726.19	Joback Method
cpg	528.32	J/mol×K	766.75	Joback Method

cpg	542.57	J/mol×K	807.31	Joback Method
cpg	555.64	J/mol×K	847.87	Joback Method
cpg	567.59	J/mol×K	888.43	Joback Method
cpg	578.49	J/mol×K	928.99	Joback Method
cpg	588.41	J/mol×K	969.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97994575&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume