1-Propanone, 1-cyclohexyl-2-hydroxy-, m-carbanilate

Inchi: InChI=1S/C16H20ClNO3/c1-11(15(19)12-6-3-2-4-7-12)21-16(20)18-14-9-5-8-13(17)10-1
InchiKey: IFWQOOWEAXAQLP-UHFFFAOYSA-N
Formula: C16H20ClNO3
SMILES: CC(OC(=O)Nc1cccc(Cl)c1)C(=O)C1CCCCC1
Mol. weight [g/mol]: 309.79

Physical Properties

Property code	Value	Unit	Source
gf	-76.75	kJ/mol	Joback Method
hf	-419.12	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.426		Crippen Method
mcvol	232.910	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	834.01	K	Joback Method
tc	1071.24	K	Joback Method
tf	506.07	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.70	J/mol×K	834.01	Joback Method
cpg	711.77	J/mol×K	873.55	Joback Method
cpg	725.39	J/mol×K	913.09	Joback Method
cpg	737.63	J/mol×K	952.62	Joback Method
cpg	748.52	J/mol×K	992.16	Joback Method
cpg	758.13	J/mol×K	1031.70	Joback Method
cpg	766.50	J/mol×K	1071.24	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=B6007926&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume