3'-chloro,4'-methylenanthoanilide

Inchi: InChI=1S/C14H20ClNO/c1-3-4-5-6-7-14(17)16-12-9-8-11(2)13(15)10-12/h8-10H,3-7H2,1
InchiKey: JHJJKXRETOKFNP-UHFFFAOYSA-N
Formula: C14H20ClNO
SMILES: CCCCCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 253.77

Physical Properties

Property code	Value	Unit	Source
gf	108.69	kJ/mol	Joback Method
hf	-193.55	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.557		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	2132.00		NIST Webbook
tb	697.83	K	Joback Method
tc	905.24	K	Joback Method
tf	431.51	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.39	J/mol×K	697.83	Joback Method
cpg	564.19	J/mol×K	732.40	Joback Method
cpg	578.10	J/mol×K	766.97	Joback Method
cpg	591.15	J/mol×K	801.53	Joback Method
cpg	603.37	J/mol×K	836.10	Joback Method
cpg	614.80	J/mol×K	870.67	Joback Method
cpg	625.48	J/mol×K	905.24	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=R149136&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume