3'-chloro,4'-methylpelargoanilide

Inchi: InChI=1S/C16H24ClNO/c1-3-4-5-6-7-8-9-16(19)18-14-11-10-13(2)15(17)12-14/h10-12H,
InchiKey: UWVWDJSGXYBBLV-UHFFFAOYSA-N
Formula: C16H24ClNO
SMILES: CCCCCCCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 281.82

Physical Properties

Property code	Value	Unit	Source
gf	125.53	kJ/mol	Joback Method
hf	-234.83	kJ/mol	Joback Method
hfus	41.35	kJ/mol	Joback Method
hvap	72.38	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.338		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2329.00		NIST Webbook
tb	743.59	K	Joback Method
tc	946.46	K	Joback Method
tf	454.05	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.88	J/mol×K	743.59	Joback Method
cpg	673.44	J/mol×K	777.40	Joback Method
cpg	688.07	J/mol×K	811.21	Joback Method
cpg	701.80	J/mol×K	845.02	Joback Method
cpg	714.68	J/mol×K	878.84	Joback Method
cpg	726.73	J/mol×K	912.65	Joback Method
cpg	738.01	J/mol×K	946.46	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=R149141&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