2-(2-propynylamino)-5-chloro-benzophenone

Inchi: InChI=1S/C16H12ClNO/c1-2-10-18-15-9-8-13(17)11-14(15)16(19)12-6-4-3-5-7-12/h1,3-9
InchiKey: TXZMSINCINMNAL-UHFFFAOYSA-N
Formula: C16H12ClNO
SMILES: C#CCNc1ccc(Cl)cc1C(=O)c1ccccc1
Mol. weight [g/mol]: 269.73

Physical Properties

Property code	Value	Unit	Source
gf	461.01	kJ/mol	Joback Method
hf	293.60	kJ/mol	Joback Method
hfus	38.37	kJ/mol	Joback Method
hvap	74.51	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	3.616		Crippen Method
mcvol	203.970	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2204.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	760.39	K	Joback Method
tc	1013.60	K	Joback Method
tf	527.44	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.79	J/mol×K	760.39	Joback Method
cpg	530.80	J/mol×K	802.59	Joback Method
cpg	542.67	J/mol×K	844.79	Joback Method
cpg	553.51	J/mol×K	886.99	Joback Method
cpg	563.40	J/mol×K	929.19	Joback Method
cpg	572.45	J/mol×K	971.39	Joback Method
cpg	580.75	J/mol×K	1013.60	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=R42554&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