but-3-yn-2-yl N-(3-chlorophenyl)carbamate

Inchi: InChI=1S/C11H10ClNO2/c1-3-8(2)15-11(14)13-10-6-4-5-9(12)7-10/h1,4-8H,2H3,(H,13,14
InchiKey: ULBXWWGWDPVHAO-UHFFFAOYSA-N
Formula: C11H10ClNO2
SMILES: C#CC(C)OC(=O)Nc1cccc(Cl)c1
Mol. weight [g/mol]: 223.66

Physical Properties

Property code	Value	Unit	Source
gf	208.69	kJ/mol	Joback Method
hf	34.24	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-2.62		Aqueous Solubility Prediction Method
logp	2.910		Crippen Method
mcvol	163.150	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	636.31	K	Joback Method
tc	869.20	K	Joback Method
tf	318.65	K	Aqueous Solubility Prediction Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.99	J/mol×K	636.31	Joback Method
cpg	391.00	J/mol×K	675.12	Joback Method
cpg	402.15	J/mol×K	713.94	Joback Method
cpg	412.46	J/mol×K	752.75	Joback Method
cpg	421.98	J/mol×K	791.57	Joback Method
cpg	430.73	J/mol×K	830.38	Joback Method
cpg	438.75	J/mol×K	869.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:
https://www.chemeo.com/cid/112-140-1/but-3-yn-2-yl-N-3-chlorophenyl-carbamate.pdf
Generated by Cheméo on 2024-04-29 00:36:24.651247413 +0000 UTC m=+16640233.571824726.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.