Buturon

Other names: 1-but-3-yn-2-yl-3-(4-chlorophenyl)-1-methylurea
Inchi: InChI=1S/C12H13ClN2O/c1-4-9(2)15(3)12(16)14-11-7-5-10(13)6-8-11/h1,5-9H,2-3H3,(H
InchiKey: BYYMILHAKOURNM-UHFFFAOYSA-N
Formula: C12H13ClN2O
SMILES: C#CC(C)N(C)C(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 236.70

Physical Properties

Property code	Value	Unit	Source
gf	432.89	kJ/mol	Joback Method
hf	213.35	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	64.32	kJ/mol	Joback Method
log10ws	-3.90		Aqueous Solubility Prediction Method
log10ws	-3.90		Estimated Solubility Method
logp	2.825		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	649.21	K	Joback Method
tc	877.15	K	Joback Method
tf	460.89	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.45	J/mol×K	649.21	Joback Method
cpg	453.83	J/mol×K	687.20	Joback Method
cpg	466.21	J/mol×K	725.19	Joback Method
cpg	477.66	J/mol×K	763.18	Joback Method
cpg	488.23	J/mol×K	801.17	Joback Method
cpg	498.00	J/mol×K	839.16	Joback Method

cpg	507.03	J/mol×K	877.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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