Acetamide, N-[2-acetoxy-3-(2-cyanophenyloxy)propyl]-

Other names: Bunitrolol desisobutyl, acetylated
Inchi: InChI=1S/C14H16N2O4/c1-10(17)16-8-13(20-11(2)18)9-19-14-6-4-3-5-12(14)7-15/h3-6,1
InchiKey: MOEZTTXOWMBABA-UHFFFAOYSA-N
Formula: C14H16N2O4
SMILES: CC(=O)NCC(COc1ccccc1C#N)OC(C)=O
Mol. weight [g/mol]: 276.29

Physical Properties

Property code	Value	Unit	Source
gf	-77.93	kJ/mol	Joback Method
hf	-383.76	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	84.53	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.005		Crippen Method
mcvol	210.600	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	2040.00		NIST Webbook
rinpol	2040.00		NIST Webbook
tb	855.77	K	Joback Method
tc	1077.38	K	Joback Method
tf	533.45	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.50	J/mol×K	855.77	Joback Method
cpg	623.33	J/mol×K	892.71	Joback Method
cpg	633.13	J/mol×K	929.64	Joback Method
cpg	641.91	J/mol×K	966.58	Joback Method
cpg	649.68	J/mol×K	1003.51	Joback Method
cpg	656.44	J/mol×K	1040.45	Joback Method
cpg	662.22	J/mol×K	1077.38	Joback Method

Sources

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=U280825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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