2-Acetylamino-6-methoxy-naphthalene

Inchi: InChI=1S/C13H13NO2/c1-9(15)14-12-5-3-11-8-13(16-2)6-4-10(11)7-12/h3-8H,1-2H3,(H,
InchiKey: ZAHHHOXQHKERLZ-UHFFFAOYSA-N
Formula: C13H13NO2
SMILES: COc1ccc2cc(NC(C)=O)ccc2c1
Mol. weight [g/mol]: 215.25
CAS: 3900-46-7

Physical Properties

Property code	Value	Unit	Source
gf	113.85	kJ/mol	Joback Method
hf	-98.32	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	65.36	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.807		Crippen Method
mcvol	168.230	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	678.92	K	Joback Method
tc	908.47	K	Joback Method
tf	445.25	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.76	J/mol×K	678.92	Joback Method
cpg	446.11	J/mol×K	717.18	Joback Method
cpg	458.53	J/mol×K	755.44	Joback Method
cpg	470.06	J/mol×K	793.70	Joback Method
cpg	480.75	J/mol×K	831.95	Joback Method
cpg	490.65	J/mol×K	870.21	Joback Method
cpg	499.81	J/mol×K	908.47	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=C3900467&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume