pelletierine

Inchi: InChI=1S/C8H15NO/c1-7(10)6-8-4-2-3-5-9-8/h8-9H,2-6H2,1H3
InchiKey: JEIZLWNUBXHADF-UHFFFAOYSA-N
Formula: C8H15NO
SMILES: CC(=O)CC1CCCCN1
Mol. weight [g/mol]: 141.21

Physical Properties

Property code	Value	Unit	Source
gf	-0.28	kJ/mol	Joback Method
hf	-228.90	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-0.45		Aqueous Solubility Prediction Method
logp	1.108		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
tb	504.41	K	Joback Method
tc	723.81	K	Joback Method
tf	342.26	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.80	J/mol×K	504.41	Joback Method
cpg	298.44	J/mol×K	540.98	Joback Method
cpg	314.20	J/mol×K	577.54	Joback Method
cpg	329.09	J/mol×K	614.11	Joback Method
cpg	343.13	J/mol×K	650.68	Joback Method
cpg	356.34	J/mol×K	687.24	Joback Method
cpg	368.73	J/mol×K	723.81	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

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