6-ethyl-1,2,3,4,5,6-hexahydro-7H-cyclopenta[b]py

Inchi: InChI=1S/C10H15NO/c1-2-7-6-8-4-3-5-11-9(8)10(7)12/h7,11H,2-6H2,1H3
InchiKey: GOTCNQZLHJWEAK-UHFFFAOYSA-N
Formula: C10H15NO
SMILES: CCC1CC2=C(NCCC2)C1=O
Mol. weight [g/mol]: 165.23

Physical Properties

Property code	Value	Unit	Source
gf	102.05	kJ/mol	Joback Method
hf	-167.32	kJ/mol	Joback Method
hfus	20.10	kJ/mol	Joback Method
hvap	51.13	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.623		Crippen Method
mcvol	137.290	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	584.65	K	Joback Method
tc	823.82	K	Joback Method
tf	431.07	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.21	J/mol×K	584.65	Joback Method
cpg	368.78	J/mol×K	624.51	Joback Method
cpg	385.32	J/mol×K	664.37	Joback Method
cpg	400.85	J/mol×K	704.24	Joback Method
cpg	415.38	J/mol×K	744.10	Joback Method
cpg	428.94	J/mol×K	783.96	Joback Method
cpg	441.54	J/mol×K	823.82	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=R225186&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