3-Piperidinecarbamic acid, 2,6-dioxo-, benzyl ester, (dl)

Inchi: InChI=1S/C13H14N2O4/c16-11-7-6-10(12(17)15-11)14-13(18)19-8-9-4-2-1-3-5-9/h1-5,10

InchiKey: JJFWWAGUYKLJRN-UHFFFAOYSA-N

Formula: C13H14N2O4

SMILES: O=C1CCC(NC(=O)OCc2ccccc2)C(=O)N1

Mol. weight [g/mol]: 262.26

CAS: 24666-55-5

Physical Properties

Property code	Value	Unit	Source
gf	-106.56	kJ/mol	Joback Method
hf	-449.72	kJ/mol	Joback Method
hfus	31.80	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	0.718		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
tb	853.72	K	Joback Method
tc	1112.31	K	Joback Method
tf	636.36	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.78	J/mol×K	853.72	Joback Method
cpg	605.55	J/mol×K	896.82	Joback Method
cpg	617.36	J/mol×K	939.92	Joback Method
cpg	627.16	J/mol×K	983.01	Joback Method
cpg	634.87	J/mol×K	1026.11	Joback Method
cpg	640.45	J/mol×K	1069.21	Joback Method
cpg	643.81	J/mol×K	1112.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C24666555&Units=SI

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