

(2,6-Dioxo-4-piperidinyl)acetic acid

Inchi:	InChI=1S/C7H9NO4/c9-5-1-4(3-7(11)12)2-6(10)8-5/h4H,1-3H2,(H,11,12)(H,8,9,10)
InchiKey:	MLOIZNBOQITCOX-UHFFFAOYSA-N
Formula:	C7H9NO4
SMILES:	O=C(O)CC1CC(=O)NC(=O)C1
Mol. weight [g/mol]:	171.15
CAS:	6258-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-390.70	kJ/mol	Joback Method
hf	-635.89	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	70.28	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	-0.486		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	709.35	K	Joback Method
tc	940.09	K	Joback Method
tf	528.25	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.15	J/molxK	709.35	Joback Method
cpg	349.07	J/molxK	747.81	Joback Method
cpg	360.11	J/molxK	786.26	Joback Method
cpg	370.21	J/molxK	824.72	Joback Method
cpg	379.32	J/molxK	863.18	Joback Method
cpg	387.36	J/molxK	901.63	Joback Method
cpg	394.29	J/molxK	940.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6258282&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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