3-((4-Hydroxyphenyl)-methyl)-2,5-piperazinedione

Inchi: InChI=1S/C11H12N2O3/c14-8-3-1-7(2-4-8)5-9-11(16)12-6-10(15)13-9/h1-4,9,14H,5-6H2
InchiKey: QHLSAVHDWSYPEP-UHFFFAOYSA-N
Formula: C11H12N2O3
SMILES: O=C1CNC(=O)C(Cc2ccc(O)cc2)N1
Mol. weight [g/mol]: 220.22
CAS: 5845-66-9

Physical Properties

Property code	Value	Unit	Source
chs	-5531.20 ± 0.40	kJ/mol	NIST Webbook
gf	-45.78	kJ/mol	Joback Method
hf	-356.61	kJ/mol	Joback Method
hfus	34.10	kJ/mol	Joback Method
hvap	77.81	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	-0.451		Crippen Method
mcvol	160.200	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
tb	810.67	K	Joback Method
tc	1092.30	K	Joback Method
tf	705.75	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.59	J/mol×K	810.67	Joback Method
cpg	500.52	J/mol×K	857.61	Joback Method
cpg	513.92	J/mol×K	904.55	Joback Method
cpg	525.81	J/mol×K	951.48	Joback Method
cpg	536.18	J/mol×K	998.42	Joback Method
cpg	545.02	J/mol×K	1045.36	Joback Method
cpg	552.34	J/mol×K	1092.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5845669&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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