

Isophthalamide

Other names:	1,3-Benzenedicarboxamide isophthaldiamide
Inchi:	InChI=1S/C8H8N2O2/c9-7(11)5-2-1-3-6(4-5)8(10)12/h1-4H,(H2,9,11)(H2,10,12)
InchiKey:	QZUPTXGVPYNUIT-UHFFFAOYSA-N
Formula:	C8H8N2O2
SMILES:	NC(=O)c1cccc(C(N)=O)c1
Mol. weight [g/mol]:	164.16
CAS:	1740-57-4

Physical Properties

Property code	Value	Unit	Source
chs	-3854.60 ± 0.96	kJ/mol	NIST Webbook
gf	-5.68	kJ/mol	Joback Method
hf	-382.00 ± 0.40	kJ/mol	NIST Webbook
hfs	-436.90 ± 1.00	kJ/mol	NIST Webbook
hfus	23.72	kJ/mol	Joback Method
hsub	54.40 ± 4.20	kJ/mol	NIST Webbook
hvap	71.11	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	-0.116		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
tb	666.90	K	Joback Method
tc	914.95	K	Joback Method
tf	485.24	K	Joback Method
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.26	J/mol×K	666.90	Joback Method
cpg	312.95	J/mol×K	708.24	Joback Method
cpg	321.83	J/mol×K	749.58	Joback Method
cpg	329.94	J/mol×K	790.92	Joback Method

cpg	337.31	J/mol×K	832.27	Joback Method
cpg	343.99	J/mol×K	873.61	Joback Method
cpg	350.01	J/mol×K	914.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1740574&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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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

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