Terephthalamide

Other names:	p-Carbamoylbenzamide
	p-Phthalamide
	Terephthalamimidic acid
	Terephthaldiamide
	Terephthalic acid diamide
	Terephthalic diamide
	1,4-Benzenedicarboxamide
Inchi:	InChI=1S/C8H8N2O2/c9-7(11)5-1-2-6(4-3-5)8(10)12/h1-4H,(H2,9,11)(H2,10,12)
InchiKey:	MHSKRLJMQQNJNC-UHFFFAOYSA-N
Formula:	C8H8N2O2
SMILES:	NC(=O)c1ccc(C(N)=O)cc1
Mol. weight [g/mol]:	164.16
CAS:	3010-82-0

Physical Properties

Property code	Value	Unit	Source
chs	-3858.30 ± 1.20	kJ/mol	NIST Webbook
gf	-5.68	kJ/mol	Joback Method
hf	-376.00 ± 4.20	kJ/mol	NIST Webbook
hfs	-433.10 ± 1.30	kJ/mol	NIST Webbook
hfus	23.72	kJ/mol	Joback Method
hsub	57.30 ± 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
hsubt	57.30 ± 4.20	kJ/mol	435.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3010820&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

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
hsubt: Enthalpy of sublimation at a given temperature
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