TEREPHTHALIC ACID DIHYDRAZIDE

Other names:	1,4-Benzenedicarboxylic acid, dihydrazide
	Terephthalic acid bishydrazide
	Terephthalic acid hydrazide
	Terephthalic hydrazide
	Terephthalohydrazide
	Terephthaloyl dihydrazide
	benzene-1,4-dicarbohydrazide
Inchi:	InChI=1S/C8H10N4O2/c9-11-7(13)5-1-2-6(4-3-5)8(14)12-10/h1-4H,9-10H2,(H,11,13)(H,1
InchiKey:	ALHNLFMSAXZKRC-UHFFFAOYSA-N
Formula:	C8H10N4O2
SMILES:	NNC(=O)c1ccc(C(=O)NN)cc1
Mol. weight [g/mol]:	194.19

Physical Properties

Property code	Value	Unit	Source
hf	-95.70	kJ/mol	Cheméo Relay (1.0)
hfus	33.92	kJ/mol	Joback Method
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-2.29		Aqueous Solubility Prediction Method
logp	-1.106		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
tb	613.19	K	Cheméo Relay (1.0)
tf	496.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.16	J/mol×K	767.24	Joback Method
cpg	401.31	J/mol×K	807.53	Joback Method
cpg	409.62	J/mol×K	847.83	Joback Method
cpg	417.15	J/mol×K	888.12	Joback Method
cpg	423.92	J/mol×K	928.41	Joback Method
cpg	429.99	J/mol×K	968.70	Joback Method

cpg	435.40	J/mol×K	1009.00	Joback Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C136641&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point