

Isovaleric acid, 2-(2,4-dinitrophenyl) hydrazide

Inchi:	InChI=1S/C11H14N4O5/c1-7(2)5-11(16)13-12-9-4-3-8(14(17)18)6-10(9)15(19)20/h3-4,6
InchiKey:	OQLCROFYRNVRAS-UHFFFAOYSA-N
Formula:	C11H14N4O5
SMILES:	CC(C)CC(=O)NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	282.25
CAS:	38562-54-8

Physical Properties

Property code	Value	Unit	Source
gf	253.41	kJ/mol	Joback Method
hf	-89.22	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	96.09	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	1.992		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
tb	945.17	K	Joback Method
tc	1198.11	K	Joback Method
tf	692.66	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.28	J/molxK	945.17	Joback Method
cpg	615.46	J/molxK	987.33	Joback Method
cpg	623.65	J/molxK	1029.48	Joback Method
cpg	630.93	J/molxK	1071.64	Joback Method
cpg	637.36	J/molxK	1113.80	Joback Method
cpg	643.01	J/molxK	1155.95	Joback Method
cpg	647.93	J/molxK	1198.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38562548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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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