

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

Inchi:	InChI=1S/C10H12N4O5/c1-6(2)10(15)12-11-8-4-3-7(13(16)17)5-9(8)14(18)19/h3-6,11H,
InchiKey:	MZMAYJWVQDIJDO-UHFFFAOYSA-N
Formula:	C10H12N4O5
SMILES:	CC(C)C(=O)NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	268.23
CAS:	7461-93-0

Physical Properties

Property code	Value	Unit	Source
gf	244.99	kJ/mol	Joback Method
hf	-68.58	kJ/mol	Joback Method
hfus	45.91	kJ/mol	Joback Method
hvap	93.87	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	1.602		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	922.29	K	Joback Method
tc	1179.08	K	Joback Method
tf	681.39	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.09	J/molxK	922.29	Joback Method
cpg	559.94	J/molxK	965.09	Joback Method
cpg	567.81	J/molxK	1007.89	Joback Method
cpg	574.77	J/molxK	1050.69	Joback Method
cpg	580.88	J/molxK	1093.48	Joback Method
cpg	586.21	J/molxK	1136.28	Joback Method
cpg	590.81	J/molxK	1179.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7461930&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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