2,4-dinitrophenylhydrazone 2-ethylbutanal

Inchi: InChI=1S/C12H16N4O4/c1-3-9(4-2)8-13-14-11-6-5-10(15(17)18)7-12(11)16(19)20/h5-9,1
InchiKey: PJQWUVGTXBCLCM-UHFFFAOYSA-N
Formula: C12H16N4O4
SMILES: CCC(C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])CC
Mol. weight [g/mol]: 280.28

Physical Properties

Property code	Value	Unit	Source
hf	31.47	kJ/mol	Joback Method
hvap	88.45	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.337		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook
tb	940.69	K	Joback Method
tc	1197.77	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139629&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

hf: Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature