N-(2,4-DINITROPHENYL)-N'-(1-METHYLPROPYLID

Inchi: InChI=1S/C10H12N4O4/c1-3-7(2)11-12-9-5-4-8(13(15)16)6-10(9)14(17)18/h4-6,12H,3H2
InchiKey: WPWSANGSIWAACK-UHFFFAOYSA-N
Formula: C10H12N4O4
SMILES: CCC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 252.23

Physical Properties

Property code	Value	Unit	Source
hf	124.33	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-3.39		Cheméo Relay (1.0)
logp	2.701		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
rinpol	2356.00		NIST Webbook
rinpol	2325.80		NIST Webbook
rinpol	2325.80		NIST Webbook
tb	586.11	K	Cheméo Relay (1.0)
tf	400.98	K	Cheméo Relay (1.0)

Sources

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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C958601&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point