

Methyl 2,6-dimethoxy-3-nitrobenzoic acid

Inchi: InChI=1S/C10H11NO6/c1-15-7-5-4-6(11(13)14)9(16-2)8(7)10(12)17-3/h4-5H,1-3H3
InchiKey: HVVQDBFINNUQBK-UHFFFAOYSA-N
Formula: C10H11NO6
SMILES: COC(=O)c1c(OC)ccc([N+](=O)[O-])c1OC
Mol. weight [g/mol]: 241.20

Physical Properties

Property code	Value	Unit	Source
hf	-554.00	kJ/mol	Cheméo Relay (1.0)
hfus	32.64	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-2.90		Cheméo Relay (1.0)
logp	1.399		Crippen Method
mcvol	164.600	ml/mol	McGowan Method
tb	582.20	K	Cheméo Relay (1.0)
tf	340.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.70	J/mol×K	724.92	Joback Method
cpg	449.28	J/mol×K	763.36	Joback Method
cpg	459.92	J/mol×K	801.80	Joback Method
cpg	469.61	J/mol×K	840.24	Joback Method
cpg	478.31	J/mol×K	878.68	Joback Method
cpg	485.99	J/mol×K	917.13	Joback Method
cpg	492.61	J/mol×K	955.57	Joback Method

Sources

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=C55776200&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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization 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

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