Alpha-(dimethylamino)-4,6-dinitro-o-cresol

Inchi: InChI=1S/C9H11N3O5/c1-10(2)5-6-3-7(11(14)15)4-8(9(6)13)12(16)17/h3-4,13H,5H2,1-2
InchiKey: DMNVKQMHEBSETA-UHFFFAOYSA-N
Formula: C9H11N3O5
SMILES: CN(C)Cc1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 241.20
CAS: 69245-80-3

Physical Properties

Property code	Value	Unit	Source
gf	145.31	kJ/mol	Joback Method
hf	-146.80	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.270		Crippen Method
mcvol	164.600	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	838.70	K	Joback Method
tc	1100.25	K	Joback Method
tf	674.06	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.42	J/mol×K	838.70	Joback Method
cpg	486.65	J/mol×K	882.29	Joback Method
cpg	496.34	J/mol×K	925.88	Joback Method
cpg	505.62	J/mol×K	969.47	Joback Method
cpg	514.63	J/mol×K	1013.06	Joback Method
cpg	523.53	J/mol×K	1056.66	Joback Method
cpg	532.44	J/mol×K	1100.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C69245803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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