Benzene, 1-methyl-4-(1-methylethyl)-2-nitro-

Other names:	2-Nitro-p-cymene
	p-Cymene, 2-nitro-
	2-Nitro-para-cymene
	4-Isopropyl-2-nitrotoluene
	Methyl-4-isopropyl-2-nitro-benzene
	2-Nitro-4-isopropyltoluene
Inchi:	InChI=1S/C10H13NO2/c1-7(2)9-5-4-8(3)10(6-9)11(12)13/h4-7H,1-3H3
InchiKey:	DRKFWQDBPGTSOO-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	Cc1ccc(C(C)C)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	179.22
CAS:	943-15-7

Physical Properties

Property code	Value	Unit	Source
gf	159.58	kJ/mol	Joback Method
hf	-52.18	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	57.66	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.027		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
tb	616.24	K	Joback Method
tc	856.97	K	Joback Method
tf	382.53	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.92	J/mol×K	816.85	Joback Method
cpg	357.61	J/mol×K	616.24	Joback Method
cpg	371.70	J/mol×K	656.36	Joback Method

cpg	384.84	J/mol×K	696.48	Joback Method
cpg	397.06	J/mol×K	736.61	Joback Method
cpg	408.41	J/mol×K	776.73	Joback Method
cpg	428.63	J/mol×K	856.97	Joback Method
hvapt	67.70	kJ/mol	392.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C943157&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
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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