

Acetanilide, 2-methyl-3-nitro-6-tert-butyl-

Inchi:	InChI=1S/C13H18N2O3/c1-8-11(15(17)18)7-6-10(13(3,4)5)12(8)14-9(2)16/h6-7H,1-5H3,
InchiKey:	AQEIPGBKYYXLBK-UHFFFAOYSA-N
Formula:	C13H18N2O3
SMILES:	CC(=O)Nc1c(C(C)(C)C)ccc([N+](=O)[O-])c1C
Mol. weight [g/mol]:	250.29

Physical Properties

Property code	Value	Unit	Source
gf	140.96	kJ/mol	Joback Method
hf	-188.15	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	77.27	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.159		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
tb	791.11	K	Joback Method
tc	1029.84	K	Joback Method
tf	548.87	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.11	J/molxK	791.11	Joback Method
cpg	589.55	J/molxK	830.90	Joback Method
cpg	601.95	J/molxK	870.69	Joback Method
cpg	613.38	J/molxK	910.48	Joback Method
cpg	623.93	J/molxK	950.26	Joback Method
cpg	633.66	J/molxK	990.05	Joback Method
cpg	642.64	J/molxK	1029.84	Joback Method

Sources

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=B6009294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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