

2,3,5-Trinitronaphthalene

Inchi:	InChI=1S/C10H5N3O6/c14-11(15)8-3-1-2-6-4-9(12(16)17)10(13(18)19)5-7(6)8/h1-5H
InchiKey:	ULFPAUMLKAKADU-UHFFFAOYSA-N
Formula:	C10H5N3O6
SMILES:	O=[N+]([O-])c1cc2cccc([N+](=O)[O-])c2cc1[N+](=O)[O-]
Mol. weight [g/mol]:	263.16
CAS:	87185-24-8

Physical Properties

Property code	Value	Unit	Source
gf	330.14	kJ/mol	Joback Method
hf	111.18	kJ/mol	Joback Method
hfus	45.63	kJ/mol	Joback Method
hvap	93.53	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	2.564		Crippen Method
mcvol	160.800	ml/mol	McGowan Method
pc	3853.09	kPa	Joback Method
rinpol	400.61		NIST Webbook
rinpol	400.61		NIST Webbook
tb	944.32	K	Joback Method
tc	1242.96	K	Joback Method
tf	729.97	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.08	J/molxK	944.32	Joback Method
cpg	454.65	J/molxK	994.09	Joback Method
cpg	461.58	J/molxK	1043.87	Joback Method
cpg	468.02	J/molxK	1093.64	Joback Method
cpg	474.12	J/molxK	1143.42	Joback Method
cpg	480.03	J/molxK	1193.19	Joback Method
cpg	485.89	J/molxK	1242.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87185248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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