

1,3,5-Tripicrylbenzene

Inchi:	InChI=1S/C24H9N9O18/c34-25(35)13-4-16(28(40)41)22(17(5-13)29(42)43)10-1-11(23-1
InchiKey:	XRORFQKOIIMHEE-UHFFFAOYSA-N
Formula:	C24H9N9O18
SMILES:	O=[N+]([O-])c1cc([N+](=O)[O-])c(-c2cc(-c3c([N+](=O)[O-])cc([N+](=O)[O-])cc3[N+](=O)[O-
Mol. weight [g/mol]:	711.38
CAS:	58505-78-5

Physical Properties

Property code	Value	Unit	Source
chs	-10486.00 ± 7.90	kJ/mol	NIST Webbook
gf	814.86	kJ/mol	Joback Method
hf	184.42	kJ/mol	Joback Method
hfs	-244.00 ± 17.00	kJ/mol	NIST Webbook
hfus	132.05	kJ/mol	Joback Method
hvap	234.72	kJ/mol	Joback Method
log10ws	-15.14		Crippen Method
logp	5.861		Crippen Method
mcvol	410.760	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
tb	2276.58	K	Joback Method
tc	2929.34	K	Joback Method
tf	1896.13	K	Joback Method
vc	1.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.59	J/molxK	2276.58	Joback Method
cpg	1306.41	J/molxK	2385.37	Joback Method
cpg	1362.24	J/molxK	2494.17	Joback Method
cpg	1435.24	J/molxK	2602.96	Joback Method
cpg	1527.59	J/molxK	2711.75	Joback Method
cpg	1641.45	J/molxK	2820.54	Joback Method
cpg	1778.99	J/molxK	2929.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58505785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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