

Mannitol, hexanitrate

Inchi:	InChI=1S/C6H8N6O18/c13-7(14)25-1-3(27-9(17)18)5(29-11(21)22)6(30-12(23)24)4(28-1
InchiKey:	DGMJZELBSFOPHH-UHFFFAOYSA-N
Formula:	C6H8N6O18
SMILES:	O=[N+]([O-])OCC(O[N+](=O)[O-])C(O[N+](=O)[O-])C(O[N+](=O)[O-])C(CO[N+](=O)[O-])O
Mol. weight [g/mol]:	452.16
CAS:	130-39-2

Physical Properties

Property code	Value	Unit	Source
chs	-2807.00	kJ/mol	NIST Webbook
chs	-2936.00	kJ/mol	NIST Webbook
gf	-426.82	kJ/mol	Joback Method
hf	-1046.17	kJ/mol	Joback Method
hfs	-708.80	kJ/mol	NIST Webbook
hfus	72.50	kJ/mol	Joback Method
hvap	141.40	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	-2.289		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	1380.48	K	Joback Method
tc	1690.63	K	Joback Method
tf	1092.42	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.20	J/molxK	1380.48	Joback Method
cpg	651.31	J/molxK	1432.17	Joback Method
cpg	625.30	J/molxK	1483.86	Joback Method
cpg	595.04	J/molxK	1535.56	Joback Method
cpg	560.40	J/molxK	1587.25	Joback Method
cpg	521.26	J/molxK	1638.94	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=C130392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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