

1,3-Propanediol, 2,2-dimethyl-, dinitrate

Other names:	Dimethylolpropane dinitrate Neopentyl glycol dinitrate 2,2-Dimethyl-1,3-propanediol, dinitrate
Inchi:	InChI=1S/C5H10N2O6/c1-5(2,3-12-6(8)9)4-13-7(10)11/h3-4H2,1-2H3
InchiKey:	KMZHSZUYWUWLOD-UHFFFAOYSA-N
Formula:	C5H10N2O6
SMILES:	CC(C)(CO[N+](=O)[O-])CO[N+](=O)[O-]
Mol. weight [g/mol]:	194.14
CAS:	26482-65-5

Physical Properties

Property code	Value	Unit	Source
chs	-2995.00	kJ/mol	NIST Webbook
gf	-144.84	kJ/mol	Joback Method
hf	-441.24	kJ/mol	Joback Method
hfus	26.39	kJ/mol	Joback Method
hvap	63.43	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	0.429		Crippen Method
mcvol	127.890	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	659.09	K	Joback Method
tc	898.68	K	Joback Method
tf	480.21	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.28	J/molxK	659.09	Joback Method
cpg	352.84	J/molxK	699.02	Joback Method
cpg	362.61	J/molxK	738.95	Joback Method
cpg	371.60	J/molxK	778.88	Joback Method
cpg	379.84	J/molxK	818.81	Joback Method

cpg	387.33	J/mol×K	858.75	Joback Method
cpg	394.11	J/mol×K	898.68	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=C26482655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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