

Dimethadione

Other names:	2,4-Oxazolidinedione, 5,5-dimethyl- AC 1198 Bay 1400Z Dimethadion DMO Eupractone 5,5-Dimethyl-2,4-oxazolidinedione 5,5-Dimethyloxazolidine-2,4-dione 5,5-Dimethyloxazolidinedione Bax 1400Z Dimethyloxazolidinedione Propazone 5,5-Dwumetylooksazolidyno-2,4-dion NSC-30152 Trimethadion, M(nor-)
Inchi:	InChI=1S/C5H7NO3/c1-5(2)3(7)6-4(8)9-5/h1-2H3,(H,6,7,8)
InchiKey:	JYJFNDQBESEHJQ-UHFFFAOYSA-N
Formula:	C5H7NO3
SMILES:	CC1(C)OC(=O)NC1=O
Mol. weight [g/mol]:	129.11
CAS:	695-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-221.31	kJ/mol	Joback Method
hf	-440.40	kJ/mol	Joback Method
hfus	12.93	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.031		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	5198.13	kPa	Joback Method
rinpol	1060.00		NIST Webbook
tb	540.46	K	Joback Method
tc	795.34	K	Joback Method
tf	448.95	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.60	J/mol×K	540.46	Joback Method
cpg	221.20	J/mol×K	582.94	Joback Method
cpg	232.30	J/mol×K	625.42	Joback Method
cpg	242.94	J/mol×K	667.90	Joback Method
cpg	253.20	J/mol×K	710.38	Joback Method
cpg	263.12	J/mol×K	752.86	Joback Method
cpg	272.75	J/mol×K	795.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C695534&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/21-819-9/Dimethadione.pdf>

Generated by Cheméo on 2025-12-20 05:56:15.130613286 +0000 UTC m=+5958372.660653955.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.