diethadione

Inchi: InChI=1S/C8H13NO3/c1-3-8(4-2)5-12-7(11)9-6(8)10/h3-5H2,1-2H3,(H,9,10,11)
InchiKey: ORTYMGHCFWKXHO-UHFFFAOYSA-N
Formula: C8H13NO3
SMILES: CCC1(CC)COC(=O)NC1=O
Mol. weight [g/mol]: 171.19
CAS: 702-54-5

Physical Properties

Property code	Value	Unit	Source
gf	-208.15	kJ/mol	Joback Method
hf	-508.48	kJ/mol	Joback Method
hfus	18.60	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.059		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1405.00		NIST Webbook
tb	613.37	K	Joback Method
tc	860.66	K	Joback Method
tf	479.24	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.67	J/mol×K	613.37	Joback Method
cpg	363.66	J/mol×K	654.59	Joback Method
cpg	378.90	J/mol×K	695.80	Joback Method
cpg	393.46	J/mol×K	737.02	Joback Method
cpg	407.37	J/mol×K	778.23	Joback Method
cpg	420.70	J/mol×K	819.45	Joback Method
cpg	433.49	J/mol×K	860.66	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=C702545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	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