Allobarbital

Other names: 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-di-2-propenyl-
5,5-Di-2-propenyl-2,4,6(1H,3H,5H)-pyrimidinetrione
5,5-Diallylbarbital
5,5-Diallylbarbituric acid
5,5-di(prop-2-enyl)-1,3-diazinane-2,4,6-trione
Allbarbital
Allobarbitone
Allybarbitural
Allylbarbitural
Alnox
Alobarbital
Barballyl
Barbidal
Barbituric acid, 5,5-diallyl-
Curral
Diadol
Dial
Dial (barbiturate)
Diallylbarbital
Diallymal
Dorm
Dormallyl
Malil
Malilum
NSC-9324
Novallyl

Inchi: InChI=1S/C10H12N2O3/c1-3-5-10(6-4-2)7(13)11-9(15)12-8(10)14/h3-4H,1-2,5-6H2,(H2,

InchiKey: FDQGNLOWMMVRQL-UHFFFAOYSA-N

Formula: C10H12N2O3

SMILES: C=CCC1(CC=C)C(=O)NC(=O)NC1=O

Mol. weight [g/mol]: 208.21

CAS: 52-43-7

Physical Properties

Property code	Value	Unit	Source
gf	35.61	kJ/mol	Joback Method

hf	-266.79	kJ/mol	Joback Method
hfus	22.34	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-1.80		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-2.08		Estimated Solubility Method
log10ws	-2.06		Aqueous Solubility Prediction Method
logp	0.491		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1606.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1575.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1595.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	741.91	K	Joback Method
tc	1005.43	K	Joback Method
tf	445.00 ± 4.00	K	NIST Webbook
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	519.41	J/mol×K	961.51	Joback Method
cpg	444.87	J/mol×K	741.91	Joback Method
cpg	461.42	J/mol×K	785.83	Joback Method
cpg	477.13	J/mol×K	829.75	Joback Method
cpg	492.02	J/mol×K	873.67	Joback Method
cpg	506.10	J/mol×K	917.59	Joback Method
cpg	531.96	J/mol×K	1005.43	Joback Method
hfust	32.31	kJ/mol	442.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52437&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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

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