

Malonanilide

Other names:	Malondianilide Malonanilide Propanediamide, N,N'-diphenyl- Malonic acid dianilide Malonic acid diphenylamide Malonic dianilide
Inchi:	InChI=1S/C15H14N2O2/c18-14(16-12-7-3-1-4-8-12)11-15(19)17-13-9-5-2-6-10-13/h1-10
InchiKey:	YYAQOJILQOVUSK-UHFFFAOYSA-N
Formula:	C15H14N2O2
SMILES:	O=C(CC(=O)Nc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]:	254.29

Physical Properties

Property code	Value	Unit	Source
hf	-153.70	kJ/mol	Cheméo Relay (1.0)
hfus	36.08	kJ/mol	Joback Method
hvap	108.66	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	2.654		Crippen Method
mcvol	197.790	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	626.51	K	Cheméo Relay (1.0)
tc	992.49	K	Cheméo Relay (1.0)
tf	436.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.03	J/mol×K	804.04	Joback Method
cpg	569.53	J/mol×K	844.23	Joback Method
cpg	580.89	J/mol×K	884.42	Joback Method
cpg	591.19	J/mol×K	924.61	Joback Method
cpg	600.52	J/mol×K	964.80	Joback Method

cpg	608.96	J/mol×K	1004.99	Joback Method
cpg	616.61	J/mol×K	1045.18	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C621103&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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