

Diphenamid

Other names:	Acetamide, N,N-dimethyl-2,2-diphenyl- Benzeneacetamide, N,N-dimethyl-«alpha»-phenyl- Benzeneacetamide, N,N-dimethyl-Â«alphaÂ»-phenyl- Dif 4 Diherbid Dimid Diphenamide Dymid Enide Enide 50 Enide 50W Fenam L-34314 Lilly 34,314 N,N-Dimethyl-2,2-diphenylacetamide N,N-Dimethyl-«alpha», «alpha»-Diphenylacetamide N,N-Dimethyl-Â«alphaÂ», Â«alphaÂ»-Diphenylacetamide N,N-Dimethyldiphenylacetamide Rideon Zarur
Inchi:	InChI=1S/C16H17NO/c1-17(2)16(18)15(13-9-5-3-6-10-13)14-11-7-4-8-12-14/h3-12,15H,
InchiKey:	QAHFOPIILNICLA-UHFFFAOYSA-N
Formula:	C16H17NO
SMILES:	CN(C)C(=O)C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	239.31
CAS:	957-51-7

Physical Properties

Property code	Value	Unit	Source
gf	288.08	kJ/mol	Joback Method
hf	49.16	kJ/mol	Joback Method
hfus	26.38	kJ/mol	Joback Method
hvap	64.16	kJ/mol	Joback Method
log10ws	-2.98		Estimated Solubility Method
log10ws	-2.98		Aqueous Solubility Prediction Method

logp	2.907		Crippen Method
mvol	200.330	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	2026.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	2015.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	2015.00		NIST Webbook
ripol	3023.00		NIST Webbook
ripol	3023.00		NIST Webbook
tb	684.71	K	Joback Method
tc	922.04	K	Joback Method
tf	407.40	K	Aqueous Solubility Prediction Method
tf	407.66 ± 0.20	K	NIST Webbook
tf	405.70 ± 0.20	K	NIST Webbook
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.72	J/mol×K	684.71	Joback Method
cpg	548.91	J/mol×K	724.26	Joback Method
cpg	564.70	J/mol×K	763.82	Joback Method
cpg	579.20	J/mol×K	803.37	Joback Method
cpg	592.50	J/mol×K	842.93	Joback Method
cpg	604.69	J/mol×K	882.48	Joback Method
cpg	615.87	J/mol×K	922.04	Joback Method
hfust	25.43	kJ/mol	407.10	NIST Webbook
hfust	25.43	kJ/mol	402.00	NIST Webbook

Sources

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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C957517&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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