

Formamide, N,N-di-(1-phenylethyl), diastereomer # 2

Inchi:	InChI=1S/C17H19NO/c1-14(16-9-5-3-6-10-16)18(13-19)15(2)17-11-7-4-8-12-17/h3-15H,
InchiKey:	FDPSAOFMNCFKOH-UHFFFAOYSA-N
Formula:	C17H19NO
SMILES:	CC(c1ccccc1)N(C=O)C(C)c1ccccc1
Mol. weight [g/mol]:	253.34

Physical Properties

Property code	Value	Unit	Source
gf	323.46	kJ/mol	Joback Method
hf	50.24	kJ/mol	Joback Method
hfus	26.13	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.967		Crippen Method
mcvol	214.420	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	701.94	K	Joback Method
tc	934.40	K	Joback Method
tf	378.66	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.61	J/molxK	701.94	Joback Method
cpg	603.10	J/molxK	740.68	Joback Method
cpg	619.20	J/molxK	779.43	Joback Method
cpg	634.02	J/molxK	818.17	Joback Method
cpg	647.64	J/molxK	856.91	Joback Method
cpg	660.17	J/molxK	895.66	Joback Method
cpg	671.70	J/molxK	934.40	Joback Method

Sources

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=R636447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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