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

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	2042.00		NIST Webbook
rinpol	2042.00		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/mol×K	701.94	Joback Method
cpg	603.10	J/mol×K	740.68	Joback Method
cpg	619.20	J/mol×K	779.43	Joback Method
cpg	634.02	J/mol×K	818.17	Joback Method
cpg	647.64	J/mol×K	856.91	Joback Method
cpg	660.17	J/mol×K	895.66	Joback Method
cpg	671.70	J/mol×K	934.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R636432&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
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