

«alpha»-methyl-N-(1-phenylethyl)-benzenethanamide

N-methyl

InChI: InChI=1S/C18H23N/c1-15(14-17-10-6-4-7-11-17)19(3)16(2)18-12-8-5-9-13-18/h4-13,15-17

InchiKey: YMFGDVWZZYVKEP-UHFFFAOYSA-N

Formula: C18H23N

SMILES: CC(Cc1ccccc1)N(C)C(C)c1ccccc1

Mol. weight [g/mol]: 253.38

Physical Properties

Property code	Value	Unit	Source
gf	431.40	kJ/mol	Joback Method
hf	115.18	kJ/mol	Joback Method
hfus	26.43	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.311		Crippen Method
mcvol	226.940	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	676.16	K	Joback Method
tc	903.13	K	Joback Method
tf	347.93	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.60	J/molxK	676.16	Joback Method
cpg	638.74	J/molxK	713.99	Joback Method
cpg	657.41	J/molxK	751.82	Joback Method
cpg	674.70	J/molxK	789.64	Joback Method
cpg	690.70	J/molxK	827.47	Joback Method
cpg	705.52	J/molxK	865.30	Joback Method
cpg	719.23	J/molxK	903.13	Joback Method

Sources

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=R279346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

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