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

Inchi: InChI=1S/C17H21N/c1-14(13-16-9-5-3-6-10-16)18-15(2)17-11-7-4-8-12-17/h3-12,14-15,
InchiKey: DVWYTXULDUSWQH-UHFFFAOYSA-N
Formula: C17H21N
SMILES: CC(Cc1ccccc1)NC(C)c1ccccc1
Mol. weight [g/mol]: 239.36

Physical Properties

Property code	Value	Unit	Source
gf	401.59	kJ/mol	Joback Method
hf	121.76	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.968		Crippen Method
mcvol	212.850	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	691.01	K	Joback Method
tc	923.93	K	Joback Method
tf	356.85	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.19	J/mol×K	691.01	Joback Method
cpg	600.94	J/mol×K	729.83	Joback Method
cpg	618.29	J/mol×K	768.65	Joback Method
cpg	634.31	J/mol×K	807.47	Joback Method
cpg	649.10	J/mol×K	846.29	Joback Method
cpg	662.75	J/mol×K	885.11	Joback Method
cpg	675.34	J/mol×K	923.93	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=R279326&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
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