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

Inchi: InChI=1S/C18H21NO/c1-15(13-17-9-5-3-6-10-17)19(14-20)16(2)18-11-7-4-8-12-18/h3-12

InchiKey: BXWRURSTCOJSEZ-UHFFFAOYSA-N

Formula: C18H21NO

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

Mol. weight [g/mol]: 267.37

Physical Properties

Property code	Value	Unit	Source
gf	331.88	kJ/mol	Joback Method
hf	29.60	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	68.20	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.837		Crippen Method
mcvol	228.510	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2169.00		NIST Webbook
tb	724.82	K	Joback Method
tc	953.03	K	Joback Method
tf	389.93	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.01	J/mol×K	724.82	Joback Method
cpg	657.66	J/mol×K	762.86	Joback Method
cpg	673.96	J/mol×K	800.89	Joback Method
cpg	688.99	J/mol×K	838.93	Joback Method
cpg	702.84	J/mol×K	876.96	Joback Method
cpg	715.63	J/mol×K	915.00	Joback Method
cpg	727.43	J/mol×K	953.03	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=R279331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume