

Benzeneacetamide, N-methyl-

Other names:	N-Methyl-2-phenylacetamide Acetamide, N-methyl-2-phenyl- N-Methylphenylacetamide
Inchi:	InChI=1S/C9H11NO/c1-10-9(11)7-8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,10,11)
InchiKey:	RKEXPBCMGJAOLM-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CNC(=O)Cc1ccccc1
Mol. weight [g/mol]:	149.19
CAS:	6830-82-6

Physical Properties

Property code	Value	Unit	Source
gf	97.78	kJ/mol	Joback Method
hf	-51.67	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	0.975		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	536.04	K	Joback Method
tc	754.91	K	Joback Method
tf	330.00 ± 3.00	K	NIST Webbook
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.38	J/molxK	536.04	Joback Method
cpg	291.41	J/molxK	572.52	Joback Method
cpg	303.61	J/molxK	609.00	Joback Method
cpg	315.00	J/molxK	645.47	Joback Method
cpg	325.61	J/molxK	681.95	Joback Method
cpg	335.50	J/molxK	718.43	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=C6830826&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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