

N-(4-Acetamido-2-methylphenyl)acetamide

Other names:	Acetamide, N,N'-(2-methyl-1,4-phenylene)bis-N,N'-(2-methyl-1,4-phenylene)bis-acetamide
Inchi:	InChI=1S/C11H14N2O2/c1-7-6-10(12-8(2)14)4-5-11(7)13-9(3)15/h4-6H,1-3H3,(H,12,14)
InchiKey:	ZYCWUKASEILJBB-UHFFFAOYSA-N
Formula:	C11H14N2O2
SMILES:	CC(=O)Nc1ccc(NC(C)=O)c(C)c1
Mol. weight [g/mol]:	206.24
CAS:	19039-27-1

Physical Properties

Property code	Value	Unit	Source
gf	55.83	kJ/mol	Joback Method
hf	-175.00	kJ/mol	Joback Method
hfus	30.91	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.912		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	2211.00		NIST Webbook
tb	695.80	K	Joback Method
tc	915.16	K	Joback Method
tf	470.37	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.84	J/mol×K	695.80	Joback Method
cpg	447.23	J/mol×K	732.36	Joback Method
cpg	458.77	J/mol×K	768.92	Joback Method
cpg	469.49	J/mol×K	805.48	Joback Method
cpg	479.43	J/mol×K	842.04	Joback Method
cpg	488.61	J/mol×K	878.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19039271&Units=SI
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

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

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