

Acetamide,N-methyl-N-(2-methylphenyl)-

Inchi:	InChI=1S/C10H13NO/c1-8-6-4-5-7-10(8)11(3)9(2)12/h4-7H,1-3H3
InchiKey:	QKIDBCKIVIQWLL-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CC(=O)N(C)c1ccccc1C
Mol. weight [g/mol]:	163.22
CAS:	29823-47-0

Physical Properties

Property code	Value	Unit	Source
gf	117.96	kJ/mol	Joback Method
hf	-69.72	kJ/mol	Joback Method
hfus	19.93	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
ie	8.82	eV	NIST Webbook
log10ws	-2.05		Crippen Method
logp	1.978		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
tb	526.17	K	Joback Method
tc	739.11	K	Joback Method
tf	323.80	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.22	J/molxK	526.17	Joback Method
cpg	324.55	J/molxK	561.66	Joback Method
cpg	338.00	J/molxK	597.15	Joback Method
cpg	350.61	J/molxK	632.64	Joback Method
cpg	362.42	J/molxK	668.13	Joback Method
cpg	373.47	J/molxK	703.62	Joback Method
cpg	383.78	J/molxK	739.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29823470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
ie:	Ionization energy
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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