[4-(Acetaminomethyl)phenyl]methanamine

Other names: N-[(4-Aminomethyl)benzyl]acetamide
N-[(4-Aminomethyl-phenyl)methyl]acetamide
Inchi: InChI=1S/C10H14N2O/c1-8(13)12-7-10-4-2-9(6-11)3-5-10/h2-5H,6-7,11H2,1H3,(H,12,13
InchiKey: LMWLRQKZZZGYDQ-UHFFFAOYSA-N
Formula: C10H14N2O
SMILES: CC(=O)NCc1ccc(CN)cc1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	163.02	kJ/mol	Joback Method
hf	-49.99	kJ/mol	Joback Method
hfus	27.20	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	0.781		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	2434.00		NIST Webbook
tb	636.43	K	Joback Method
tc	860.21	K	Joback Method
tf	427.25	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.14	J/mol×K	636.43	Joback Method
cpg	394.21	J/mol×K	673.73	Joback Method
cpg	406.42	J/mol×K	711.02	Joback Method
cpg	417.78	J/mol×K	748.32	Joback Method
cpg	428.35	J/mol×K	785.62	Joback Method
cpg	438.17	J/mol×K	822.91	Joback Method
cpg	447.26	J/mol×K	860.21	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=U373141&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

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