Pentanamide, N-(4-methoxyphenyl)-5-chloro-

Inchi: InChI=1S/C12H16ClNO2/c1-16-11-7-5-10(6-8-11)14-12(15)4-2-3-9-13/h5-8H,2-4,9H2,1H
InchiKey: FBJIABNNCRFUEM-UHFFFAOYSA-N
Formula: C12H16ClNO2
SMILES: COc1ccc(NC(=O)CCCCCl)cc1
Mol. weight [g/mol]: 241.71

Physical Properties

Property code	Value	Unit	Source
gf	-3.52	kJ/mol	Joback Method
hf	-273.02	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	65.22	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.043		Crippen Method
mcvol	185.840	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	669.51	K	Joback Method
tc	879.98	K	Joback Method
tf	418.68	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.26	J/mol×K	669.51	Joback Method
cpg	485.94	J/mol×K	704.59	Joback Method
cpg	498.77	J/mol×K	739.67	Joback Method
cpg	510.76	J/mol×K	774.74	Joback Method
cpg	521.95	J/mol×K	809.82	Joback Method
cpg	532.36	J/mol×K	844.90	Joback Method
cpg	542.00	J/mol×K	879.98	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=U307361&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