Propanamide, N-(4-methoxyphenyl)-3-chloro-

Inchi: InChI=1S/C10H12ClNO2/c1-14-9-4-2-8(3-5-9)12-10(13)6-7-11/h2-5H,6-7H2,1H3,(H,12,1
InchiKey: ZVNNQFDBJXKWOE-UHFFFAOYSA-N
Formula: C10H12ClNO2
SMILES: COc1ccc(NC(=O)CCCl)cc1
Mol. weight [g/mol]: 213.66

Physical Properties

Property code	Value	Unit	Source
gf	-20.36	kJ/mol	Joback Method
hf	-231.74	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.263		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1915.00		NIST Webbook
tb	623.75	K	Joback Method
tc	841.19	K	Joback Method
tf	396.14	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.95	J/mol×K	623.75	Joback Method
cpg	385.36	J/mol×K	659.99	Joback Method
cpg	397.00	J/mol×K	696.23	Joback Method
cpg	407.87	J/mol×K	732.47	Joback Method
cpg	418.00	J/mol×K	768.71	Joback Method
cpg	427.41	J/mol×K	804.95	Joback Method
cpg	436.11	J/mol×K	841.19	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=U307228&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