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

Inchi: InChI=1S/C9H9BrClNO/c10-7-1-3-8(4-2-7)12-9(13)5-6-11/h1-4H,5-6H2,(H,12,13)
InchiKey: VZDHQIUBGSISCC-UHFFFAOYSA-N
Formula: C9H9BrClNO
SMILES: O=C(CCCl)Nc1ccc(Br)cc1
Mol. weight [g/mol]: 262.53

Physical Properties

Property code	Value	Unit	Source
gf	90.54	kJ/mol	Joback Method
hf	-52.55	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.016		Crippen Method
mcvol	155.200	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	1964.00		NIST Webbook
rinpol	1964.00		NIST Webbook
tb	644.61	K	Joback Method
tc	881.17	K	Joback Method
tf	422.44	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.34	J/mol×K	644.61	Joback Method
cpg	345.89	J/mol×K	684.04	Joback Method
cpg	355.62	J/mol×K	723.46	Joback Method
cpg	364.58	J/mol×K	762.89	Joback Method
cpg	372.84	J/mol×K	802.31	Joback Method
cpg	380.43	J/mol×K	841.74	Joback Method
cpg	387.42	J/mol×K	881.17	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307229&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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