N-(4-bromophenyl)-2,2,3-trichloropropanamide

Inchi: InChI=1S/C9H7BrCl3NO/c10-6-1-3-7(4-2-6)14-8(15)9(12,13)5-11/h1-4H,5H2,(H,14,15)
InchiKey: MQRNPORKNQYDEL-UHFFFAOYSA-N
Formula: C9H7BrCl3NO
SMILES: O=C(Nc1ccc(Br)cc1)C(Cl)(Cl)CCl
Mol. weight [g/mol]: 331.42
CAS: 116402-42-7

Physical Properties

Property code	Value	Unit	Source
gf	69.52	kJ/mol	Joback Method
hf	-92.78	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.800		Crippen Method
mcvol	179.680	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	716.24	K	Joback Method
tc	972.35	K	Joback Method
tf	484.70	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.01	J/mol×K	716.24	Joback Method
cpg	387.66	J/mol×K	758.93	Joback Method
cpg	395.45	J/mol×K	801.61	Joback Method
cpg	402.47	J/mol×K	844.30	Joback Method
cpg	408.83	J/mol×K	886.98	Joback Method
cpg	414.65	J/mol×K	929.67	Joback Method
cpg	420.04	J/mol×K	972.35	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C116402427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume