Tetrabromophthalimide

Other names: 1H-Isoindole-1,3(2H)-dione, 4,5,6,7-tetrabromo-
Phthalimide, 3,4,5,6-tetrabromo-
3,4,5,6-Tetrabromophthalimide
Inchi: InChI=1S/C8HBr4NO2/c9-3-1-2(8(15)13-7(1)14)4(10)6(12)5(3)11/h(H,13,14,15)
InchiKey: QRFTXHFUNIFHST-UHFFFAOYSA-N
Formula: C8HBr4NO2
SMILES: O=C1NC(=O)c2c(Br)c(Br)c(Br)c(Br)c21
Mol. weight [g/mol]: 462.71
CAS: 24407-32-7

Physical Properties

Property code	Value	Unit	Source
gf	49.01	kJ/mol	Joback Method
hf	-68.40	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	3.620		Crippen Method
mcvol	172.080	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
tb	894.26	K	Joback Method
tc	1205.37	K	Joback Method
tf	771.79	K	Joback Method
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.18	J/mol×K	894.26	Joback Method
cpg	331.48	J/mol×K	946.11	Joback Method
cpg	336.97	J/mol×K	997.96	Joback Method
cpg	341.66	J/mol×K	1049.82	Joback Method
cpg	345.53	J/mol×K	1101.67	Joback Method
cpg	348.58	J/mol×K	1153.52	Joback Method

cpg	350.80	J/mol×K	1205.37	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=C24407327&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