Deltamethrin, isomer 1

Inchi: InChI=1S/C22H19Br2NO3/c1-22(2)17(12-19(23)24)20(22)21(26)28-18(13-25)14-7-6-10-
InchiKey: OWZREIFADZCYQD-IMBCPYESSA-N
Formula: C22H19Br2NO3
SMILES: CC1(C)C(C=C(Br)Br)C1C(=O)OC(C#N)c1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]: 505.20

Physical Properties

Property code	Value	Unit	Source
gf	281.52	kJ/mol	Joback Method
hf	-45.79	kJ/mol	Joback Method
hfus	45.83	kJ/mol	Joback Method
hvap	102.49	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.490		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	3029.00		NIST Webbook
tb	1095.45	K	Joback Method
tc	1365.29	K	Joback Method
tf	681.36	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.63	J/mol×K	1095.45	Joback Method
cpg	969.02	J/mol×K	1140.42	Joback Method
cpg	991.68	J/mol×K	1185.40	Joback Method
cpg	1015.94	J/mol×K	1230.37	Joback Method
cpg	1042.14	J/mol×K	1275.34	Joback Method
cpg	1070.62	J/mol×K	1320.31	Joback Method
cpg	1101.69	J/mol×K	1365.29	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R566373&Units=SI

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