2,12-Dichloro-7,7-diethyl-6H,14H-dibenzo[f,i][1,5]d

Inchi: InChI=1S/C20H18Cl2O4/c1-3-20(4-2)18(23)25-16-7-5-14(21)10-12(16)9-13-11-15(22)6-8
InchiKey: ZVJLBBCJQDYEHT-UHFFFAOYSA-N
Formula: C20H18Cl2O4
SMILES: CCC1(CC)C(=O)Oc2ccc(Cl)cc2Cc2cc(Cl)ccc2OC1=O
Mol. weight [g/mol]: 393.26

Physical Properties

Property code	Value	Unit	Source
gf	-118.50	kJ/mol	Joback Method
hf	-530.27	kJ/mol	Joback Method
hfus	42.99	kJ/mol	Joback Method
hvap	92.88	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.215		Crippen Method
mcvol	273.640	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2808.00		NIST Webbook
rinpol	2808.00		NIST Webbook
tb	1014.47	K	Joback Method
tc	1287.50	K	Joback Method
tf	698.78	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.64	J/mol×K	1014.47	Joback Method
cpg	870.26	J/mol×K	1059.97	Joback Method
cpg	886.18	J/mol×K	1105.48	Joback Method
cpg	901.56	J/mol×K	1150.98	Joback Method
cpg	916.52	J/mol×K	1196.49	Joback Method
cpg	931.23	J/mol×K	1241.99	Joback Method
cpg	945.82	J/mol×K	1287.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370195&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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