1,2-Cyclohexanedicarboxylic acid, di(4-bromophenyl) ester

Inchi: InChI=1S/C20H18Br2O4/c21-13-5-9-15(10-6-13)25-19(23)17-3-1-2-4-18(17)20(24)26-16
InchiKey: XXZPHKWQZIFJGC-UHFFFAOYSA-N
Formula: C20H18Br2O4
SMILES: O=C(Oc1ccc(Br)cc1)C1CCCCC1C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 482.16

Physical Properties

Property code	Value	Unit	Source
gf	-99.38	kJ/mol	Joback Method
hf	-408.97	kJ/mol	Joback Method
hfus	43.91	kJ/mol	Joback Method
hvap	97.29	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.529		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	3272.00		NIST Webbook
rinpol	3272.00		NIST Webbook
tb	1020.10	K	Joback Method
tc	1288.83	K	Joback Method
tf	660.10	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.04	J/mol×K	1020.10	Joback Method
cpg	848.16	J/mol×K	1064.89	Joback Method
cpg	856.57	J/mol×K	1109.68	Joback Method
cpg	863.38	J/mol×K	1154.46	Joback Method
cpg	868.65	J/mol×K	1199.25	Joback Method
cpg	872.46	J/mol×K	1244.04	Joback Method
cpg	874.91	J/mol×K	1288.83	Joback Method
dvisc	0.0002833	Pa×s	660.10	Joback Method

dvisc	0.0001859	Pa×s	720.10	Joback Method
dvisc	0.0001301	Pa×s	780.10	Joback Method
dvisc	0.0000958	Pa×s	840.10	Joback Method
dvisc	0.0000735	Pa×s	900.10	Joback Method
dvisc	0.0000583	Pa×s	960.10	Joback Method
dvisc	0.0000475	Pa×s	1020.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339634&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
dvisc:	Dynamic viscosity
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