1,2-Cyclohexanedicarboxylic acid, 4-bromophenyl isohexyl ester

Inchi: InChI=1S/C20H27BrO4/c1-14(2)6-5-13-24-19(22)17-7-3-4-8-18(17)20(23)25-16-11-9-15(

InchiKey: WPSGAXINKIMSBJ-UHFFFAOYSA-N

Formula: C20H27BrO4

SMILES: CC(C)CCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 411.33

Physical Properties

Property code	Value	Unit	Source
gf	-218.92	kJ/mol	Joback Method
hf	-665.64	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	87.53	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.140		Crippen Method
mcvol	290.420	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	921.84	K	Joback Method
tc	1153.38	K	Joback Method
tf	546.36	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.02	J/mol×K	921.84	Joback Method
cpg	932.13	J/mol×K	960.43	Joback Method
cpg	945.64	J/mol×K	999.02	Joback Method
cpg	957.58	J/mol×K	1037.61	Joback Method
cpg	968.00	J/mol×K	1076.20	Joback Method
cpg	976.94	J/mol×K	1114.79	Joback Method
cpg	984.42	J/mol×K	1153.38	Joback Method
dvisc	0.0005424	Pa×s	546.36	Joback Method

dvisc	0.0003021	Pa×s	608.94	Joback Method
dvisc	0.0001876	Pa×s	671.52	Joback Method
dvisc	0.0001264	Pa×s	734.10	Joback Method
dvisc	0.0000906	Pa×s	796.68	Joback Method
dvisc	0.0000682	Pa×s	859.26	Joback Method
dvisc	0.0000533	Pa×s	921.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339629&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

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