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

Inchi: InChI=1S/C18H23BrO4/c1-12(2)11-22-17(20)15-5-3-4-6-16(15)18(21)23-14-9-7-13(19)8-

InchiKey: ZCSZPBXBYMQQIX-UHFFFAOYSA-N

Formula: C18H23BrO4

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

Mol. weight [g/mol]: 383.28

Physical Properties

Property code	Value	Unit	Source
gf	-235.76	kJ/mol	Joback Method
hf	-624.36	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.360		Crippen Method
mcvol	262.240	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	876.08	K	Joback Method
tc	1112.05	K	Joback Method
tf	523.82	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.83	J/mol×K	876.08	Joback Method
cpg	815.15	J/mol×K	915.41	Joback Method
cpg	828.88	J/mol×K	954.74	Joback Method
cpg	841.07	J/mol×K	994.07	Joback Method
cpg	851.75	J/mol×K	1033.40	Joback Method
cpg	860.95	J/mol×K	1072.72	Joback Method
cpg	868.70	J/mol×K	1112.05	Joback Method
dvisc	0.0006711	Pa×s	523.82	Joback Method
dvisc	0.0003824	Pa×s	582.53	Joback Method

dvisc	0.0002415	Pa×s	641.24	Joback Method
dvisc	0.0001648	Pa×s	699.95	Joback Method
dvisc	0.0001193	Pa×s	758.66	Joback Method
dvisc	0.0000904	Pa×s	817.37	Joback Method
dvisc	0.0000712	Pa×s	876.08	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=U339626&Units=SI

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