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

Inchi: InChI=1S/C18H23BrO4/c1-2-3-12-22-17(20)15-6-4-5-7-16(15)18(21)23-14-10-8-13(19)9-

InchiKey: JIHVSMPVLFOEED-UHFFFAOYSA-N

Formula: C18H23BrO4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 383.28

Physical Properties

Property code	Value	Unit	Source
gf	-233.32	kJ/mol	Joback Method
hf	-619.08	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	83.47	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.504		Crippen Method
mcvol	262.240	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	2545.00		NIST Webbook
tb	876.52	K	Joback Method
tc	1109.19	K	Joback Method
tf	538.82	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.30	J/mol×K	876.52	Joback Method
cpg	860.07	J/mol×K	1070.41	Joback Method
cpg	850.83	J/mol×K	1031.63	Joback Method
cpg	840.17	J/mol×K	992.85	Joback Method
cpg	828.05	J/mol×K	954.08	Joback Method
cpg	814.43	J/mol×K	915.30	Joback Method
cpg	867.92	J/mol×K	1109.19	Joback Method
dvisc	0.0000778	Pa×s	876.52	Joback Method
dvisc	0.0000975	Pa×s	820.24	Joback Method

dvisc	0.0001264	Pa×s	763.95	Joback Method
dvisc	0.0001706	Pa×s	707.67	Joback Method
dvisc	0.0002427	Pa×s	651.39	Joback Method
dvisc	0.0003690	Pa×s	595.10	Joback Method
dvisc	0.0006124	Pa×s	538.82	Joback Method

Sources

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=U339627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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