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

Inchi: InChI=1S/C17H21BrO4/c1-2-11-21-16(19)14-5-3-4-6-15(14)17(20)22-13-9-7-12(18)8-10-

InchiKey: FWTBLERNEFIDDW-UHFFFAOYSA-N

Formula: C17H21BrO4

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

Mol. weight [g/mol]: 369.25

Physical Properties

Property code	Value	Unit	Source
gf	-241.74	kJ/mol	Joback Method
hf	-598.44	kJ/mol	Joback Method
hfus	37.20	kJ/mol	Joback Method
hvap	81.24	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.114		Crippen Method
mcvol	248.150	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	853.64	K	Joback Method
tc	1089.22	K	Joback Method
tf	527.55	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.69	J/mol×K	853.64	Joback Method
cpg	756.86	J/mol×K	892.90	Joback Method
cpg	770.52	J/mol×K	932.17	Joback Method
cpg	782.70	J/mol×K	971.43	Joback Method
cpg	793.43	J/mol×K	1010.69	Joback Method
cpg	802.73	J/mol×K	1049.95	Joback Method
cpg	810.64	J/mol×K	1089.22	Joback Method
dvisc	0.0006752	Pa×s	527.55	Joback Method

dvisc	0.0004119	Pa×s	581.90	Joback Method
dvisc	0.0002734	Pa×s	636.25	Joback Method
dvisc	0.0001936	Pa×s	690.60	Joback Method
dvisc	0.0001442	Pa×s	744.94	Joback Method
dvisc	0.0001117	Pa×s	799.29	Joback Method
dvisc	0.0000895	Pa×s	853.64	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=U339625&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