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

Inchi: InChI=1S/C19H25BrO4/c1-2-3-6-13-23-18(21)16-7-4-5-8-17(16)19(22)24-15-11-9-14(20)

InchiKey: DCMARCGMTSPYLT-UHFFFAOYSA-N

Formula: C19H25BrO4

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

Mol. weight [g/mol]: 397.30

Physical Properties

Property code	Value	Unit	Source
gf	-224.90	kJ/mol	Joback Method
hf	-639.72	kJ/mol	Joback Method
hfus	42.38	kJ/mol	Joback Method
hvap	85.69	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.894		Crippen Method
mcvol	276.330	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	899.40	K	Joback Method
tc	1129.84	K	Joback Method
tf	550.09	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.60	J/mol×K	899.40	Joback Method
cpg	917.94	J/mol×K	1091.43	Joback Method
cpg	908.81	J/mol×K	1053.03	Joback Method
cpg	898.24	J/mol×K	1014.62	Joback Method
cpg	886.21	J/mol×K	976.21	Joback Method
cpg	872.67	J/mol×K	937.81	Joback Method
cpg	925.68	J/mol×K	1129.84	Joback Method
dvisc	0.0000675	Pa×s	899.40	Joback Method

dvisc	0.0000849	Pa×s	841.18	Joback Method
dvisc	0.0001105	Pa×s	782.96	Joback Method
dvisc	0.0001500	Pa×s	724.74	Joback Method
dvisc	0.0002148	Pa×s	666.53	Joback Method
dvisc	0.0003294	Pa×s	608.31	Joback Method
dvisc	0.0005532	Pa×s	550.09	Joback Method

Sources

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=U339628&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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