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

Inchi: InChI=1S/C22H31BrO4/c1-2-3-4-5-6-9-16-26-21(24)19-10-7-8-11-20(19)22(25)27-18-14-

InchiKey: KMAOVLZXJHOARO-UHFFFAOYSA-N

Formula: C22H31BrO4

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

Mol. weight [g/mol]: 439.38

Physical Properties

Property code	Value	Unit	Source
gf	-199.64	kJ/mol	Joback Method
hf	-701.64	kJ/mol	Joback Method
hfus	50.15	kJ/mol	Joback Method
hvap	92.37	kJ/mol	Joback Method
log10ws	-7.08		Crippen Method
logp	6.065		Crippen Method
mcvol	318.600	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2945.00		NIST Webbook
tb	968.04	K	Joback Method
tc	1196.34	K	Joback Method
tf	583.90	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.07	J/mol×K	968.04	Joback Method
cpg	1050.87	J/mol×K	1006.09	Joback Method
cpg	1064.06	J/mol×K	1044.14	Joback Method
cpg	1075.69	J/mol×K	1082.19	Joback Method
cpg	1085.80	J/mol×K	1120.24	Joback Method
cpg	1094.44	J/mol×K	1158.29	Joback Method
cpg	1101.66	J/mol×K	1196.34	Joback Method
dvisc	0.0003992	Pa×s	583.90	Joback Method
dvisc	0.0002299	Pa×s	647.92	Joback Method

dvisc	0.0001462	Pa×s	711.95	Joback Method
dvisc	0.0001002	Pa×s	775.97	Joback Method
dvisc	0.0000727	Pa×s	839.99	Joback Method
dvisc	0.0000552	Pa×s	904.02	Joback Method
dvisc	0.0000435	Pa×s	968.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339631&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

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