

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

Inchi:	InChI=1S/C23H33BrO4/c1-2-3-4-5-6-7-10-17-27-22(25)20-11-8-9-12-21(20)23(26)28-19
InchiKey:	AOEGNDJRHKSQKR-UHFFFAOYSA-N
Formula:	C23H33BrO4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	453.41

Physical Properties

Property code	Value	Unit	Source
gf	-191.22	kJ/mol	Joback Method
hf	-722.28	kJ/mol	Joback Method
hfus	52.74	kJ/mol	Joback Method
hvap	94.60	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.455		Crippen Method
mcvol	332.690	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	3056.00		NIST Webbook
tb	990.92	K	Joback Method
tc	1220.17	K	Joback Method
tf	595.17	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.55	J/molxK	990.92	Joback Method
cpg	1154.13	J/molxK	1181.96	Joback Method
cpg	1145.70	J/molxK	1143.76	Joback Method
cpg	1135.78	J/molxK	1105.55	Joback Method
cpg	1124.31	J/molxK	1067.34	Joback Method
cpg	1111.26	J/molxK	1029.13	Joback Method
cpg	1161.11	J/molxK	1220.17	Joback Method
dvisc	0.0000374	Paxs	990.92	Joback Method
dvisc	0.0000476	Paxs	924.96	Joback Method

dvisc	0.0000630	Paxs	859.00	Joback Method
dvisc	0.0000871	Paxs	793.05	Joback Method
dvisc	0.0001279	Paxs	727.09	Joback Method
dvisc	0.0002027	Paxs	661.13	Joback Method
dvisc	0.0003558	Paxs	595.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U339632&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

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