1,2-Cyclohexanedicarboxylic acid, butyl 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C19H25ClO4/c1-3-4-11-23-18(21)15-7-5-6-8-16(15)19(22)24-14-9-10-17(20)13

InchiKey: MEHGQLIZAHNMKH-UHFFFAOYSA-N

Formula: C19H25ClO4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 352.85

Physical Properties

Property code	Value	Unit	Source
gf	-260.78	kJ/mol	Joback Method
hf	-693.26	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.704		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	875.65	K	Joback Method
tc	1100.61	K	Joback Method
tf	532.73	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.86	J/mol×K	875.65	Joback Method
cpg	907.06	J/mol×K	1063.11	Joback Method
cpg	897.43	J/mol×K	1025.62	Joback Method
cpg	886.31	J/mol×K	988.13	Joback Method
cpg	873.69	J/mol×K	950.64	Joback Method
cpg	859.54	J/mol×K	913.14	Joback Method
cpg	915.22	J/mol×K	1100.61	Joback Method
dvisc	0.0000747	Pa×s	875.65	Joback Method

dvisc	0.0000935	Pa×s	818.50	Joback Method
dvisc	0.0001210	Pa×s	761.34	Joback Method
dvisc	0.0001633	Pa×s	704.19	Joback Method
dvisc	0.0002325	Pa×s	647.04	Joback Method
dvisc	0.0003544	Pa×s	589.88	Joback Method
dvisc	0.0005913	Pa×s	532.73	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=U339686&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