cis-Cyclohex-4-en-1,2-dicarboxylic acid, 4-chloro-3-methylphenyl octyl ester

Inchi: InChI=1S/C23H31ClO4/c1-3-4-5-6-7-10-15-27-22(25)19-11-8-9-12-20(19)23(26)28-18-13

InchiKey: XJIFPKVWAFBEAL-UHFFFAOYSA-N

Formula: C23H31ClO4

SMILES: CCCCCCCCOC(=O)C1CC=CCC1C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 406.94

Physical Properties

Property code	Value	Unit	Source
gf	-197.14	kJ/mol	Joback Method
hf	-718.04	kJ/mol	Joback Method
hfus	52.49	kJ/mol	Joback Method
hvap	93.50	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.040		Crippen Method
mcvol	323.130	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2903.00		NIST Webbook
tb	966.33	K	Joback Method
tc	1190.96	K	Joback Method
tf	578.57	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.82	J/mol×K	966.33	Joback Method
cpg	1066.46	J/mol×K	1003.77	Joback Method
cpg	1079.46	J/mol×K	1041.21	Joback Method
cpg	1090.88	J/mol×K	1078.64	Joback Method
cpg	1100.72	J/mol×K	1116.08	Joback Method
cpg	1109.04	J/mol×K	1153.52	Joback Method
cpg	1115.85	J/mol×K	1190.96	Joback Method
dvisc	0.0003986	Pa×s	578.57	Joback Method
dvisc	0.0002328	Pa×s	643.20	Joback Method

dvisc	0.0001500	Pa×s	707.82	Joback Method
dvisc	0.0001040	Pa×s	772.45	Joback Method
dvisc	0.0000764	Pa×s	837.08	Joback Method
dvisc	0.0000586	Pa×s	901.70	Joback Method
dvisc	0.0000466	Pa×s	966.33	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=U382653&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