1,2-Cyclohexanedicarboxylic acid, butyl 2-chloroethyl ester

Inchi: InChI=1S/C14H23ClO4/c1-2-3-9-18-13(16)11-6-4-5-7-12(11)14(17)19-10-8-15/h11-12H,2

InchiKey: SGIWRAGFENWKHK-UHFFFAOYSA-N

Formula: C14H23ClO4

SMILES: CCCCOC(=O)C1CCCCC1C(=O)OCCCl

Mol. weight [g/mol]: 290.78

Physical Properties

Property code	Value	Unit	Source
gf	-396.03	kJ/mol	Joback Method
hf	-803.65	kJ/mol	Joback Method
hfus	34.69	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.918		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	724.61	K	Joback Method
tc	927.88	K	Joback Method
tf	424.92	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.19	J/mol×K	724.61	Joback Method
cpg	723.85	J/mol×K	894.00	Joback Method
cpg	711.12	J/mol×K	860.12	Joback Method
cpg	697.29	J/mol×K	826.24	Joback Method
cpg	682.36	J/mol×K	792.37	Joback Method
cpg	666.33	J/mol×K	758.49	Joback Method
cpg	735.49	J/mol×K	927.88	Joback Method
dvisc	0.0001379	Pa×s	724.61	Joback Method

dvisc	0.0001764	Pa×s	674.66	Joback Method
dvisc	0.0002348	Pa×s	624.71	Joback Method
dvisc	0.0003285	Pa×s	574.76	Joback Method
dvisc	0.0004899	Pa×s	524.82	Joback Method
dvisc	0.0007946	Pa×s	474.87	Joback Method
dvisc	0.0014440	Pa×s	424.92	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=U340042&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