

1,2-Cyclohexanedicarboxylic acid, butyl (2-chlorocyclohexyl)methyl ester

Inchi:	InChI=1S/C19H31ClO4/c1-2-3-12-23-18(21)15-9-5-6-10-16(15)19(22)24-13-14-8-4-7-11
InchiKey:	XFPHHUMJZXFZPD-UHFFFAOYSA-N
Formula:	C19H31ClO4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1Cl
Mol. weight [g/mol]:	358.90

Physical Properties

Property code	Value	Unit	Source
gf	-337.19	kJ/mol	Joback Method
hf	-872.87	kJ/mol	Joback Method
hfus	40.55	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.477		Crippen Method
mcvol	283.970	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
tb	853.89	K	Joback Method
tc	1072.59	K	Joback Method
tf	484.41	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.15	J/molxK	853.89	Joback Method
cpg	1018.41	J/molxK	1036.14	Joback Method
cpg	1006.22	J/molxK	999.69	Joback Method
cpg	992.32	J/molxK	963.24	Joback Method
cpg	976.68	J/molxK	926.79	Joback Method
cpg	959.30	J/molxK	890.34	Joback Method
cpg	1028.91	J/molxK	1072.59	Joback Method
dvisc	0.0000945	Paxs	853.89	Joback Method
dvisc	0.0001215	Paxs	792.31	Joback Method
dvisc	0.0001629	Paxs	730.73	Joback Method

dvisc	0.0002307	Paxs	669.15	Joback Method
dvisc	0.0003504	Paxs	607.57	Joback Method
dvisc	0.0005850	Paxs	545.99	Joback Method
dvisc	0.0011124	Paxs	484.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339860&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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