

Isophthalic acid, (2-chlorocyclohexyl)methyl propyl ester

Inchi:	InChI=1S/C18H23ClO4/c1-2-10-22-17(20)13-7-5-8-14(11-13)18(21)23-12-15-6-3-4-9-16
InchiKey:	DBSSYZFDKJBEGH-UHFFFAOYSA-N
Formula:	C18H23ClO4
SMILES:	CCCOC(=O)c1cccc(C(=O)OCC2CCCCC2Cl)c1
Mol. weight [g/mol]:	338.83

Physical Properties

Property code	Value	Unit	Source
gf	-259.57	kJ/mol	Joback Method
hf	-661.15	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.208		Crippen Method
mvol	256.980	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
tb	847.79	K	Joback Method
tc	1074.08	K	Joback Method
tf	508.94	K	Joback Method
vc	0.965	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.53	J/mol×K	847.79	Joback Method
cpg	802.40	J/mol×K	885.51	Joback Method
cpg	816.77	J/mol×K	923.22	Joback Method
cpg	829.65	J/mol×K	960.94	Joback Method
cpg	841.06	J/mol×K	998.65	Joback Method
cpg	851.03	J/mol×K	1036.37	Joback Method
cpg	859.58	J/mol×K	1074.08	Joback Method
dvisc	0.0007421	Paxs	508.94	Joback Method
dvisc	0.0004307	Paxs	565.41	Joback Method
dvisc	0.0002760	Paxs	621.89	Joback Method

dvisc	0.0001904	Paxs	678.37	Joback Method
dvisc	0.0001391	Paxs	734.84	Joback Method
dvisc	0.0001063	Paxs	791.32	Joback Method
dvisc	0.0000842	Paxs	847.79	Joback Method

Sources

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=U343793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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