

Isophthalic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi:	InChI=1S/C19H19ClO4/c1-12(2)11-23-18(21)14-5-4-6-15(10-14)19(22)24-16-7-8-17(20)
InchiKey:	ZXWMMGHJLWLQFH-UHFFFAOYSA-N
Formula:	C19H19ClO4
SMILES:	<chem>Cc1cc(OC(=O)c2cccc(C(=O)OCC(C)C)c2)ccc1Cl</chem>
Mol. weight [g/mol]:	346.81

Physical Properties

Property code	Value	Unit	Source
gf	-177.18	kJ/mol	Joback Method
hf	-507.46	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	86.73	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.680		Crippen Method
mcvol	258.170	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	2737.00		NIST Webbook
tb	891.99	K	Joback Method
tc	1125.54	K	Joback Method
tf	553.53	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.42	J/molxK	891.99	Joback Method
cpg	795.64	J/molxK	1086.61	Joback Method
cpg	788.13	J/molxK	1047.69	Joback Method
cpg	779.38	J/molxK	1008.76	Joback Method
cpg	769.36	J/molxK	969.84	Joback Method
cpg	758.05	J/molxK	930.91	Joback Method
cpg	801.95	J/molxK	1125.54	Joback Method
dvisc	0.0000530	Paxs	891.99	Joback Method
dvisc	0.0000663	Paxs	835.58	Joback Method

dvisc	0.0000856	Paxs	779.17	Joback Method
dvisc	0.0001152	Paxs	722.76	Joback Method
dvisc	0.0001628	Paxs	666.35	Joback Method
dvisc	0.0002455	Paxs	609.94	Joback Method
dvisc	0.0004025	Paxs	553.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344590&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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