

Dimethyl 5-chloroisophthalate

Inchi:	InChI=1S/C10H9ClO4/c1-14-9(12)6-3-7(10(13)15-2)5-8(11)4-6/h3-5H,1-2H3
InchiKey:	CMMPMNSOVLQGMJ-UHFFFAOYSA-N
Formula:	C10H9ClO4
SMILES:	<chem>COC(=O)c1cc(Cl)cc(C(=O)OC)c1</chem>
Mol. weight [g/mol]:	228.63
CAS:	20330-90-9

Physical Properties

Property code	Value	Unit	Source
gf	-353.30	kJ/mol	Joback Method
hf	-541.48	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.913		Crippen Method
mcvol	155.120	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	654.85	K	Joback Method
tc	878.19	K	Joback Method
tf	428.16	K	Joback Method
vc	0.585	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.79	J/molxK	654.85	Joback Method
cpg	371.67	J/molxK	692.07	Joback Method
cpg	381.85	J/molxK	729.30	Joback Method
cpg	391.33	J/molxK	766.52	Joback Method
cpg	400.08	J/molxK	803.75	Joback Method
cpg	408.11	J/molxK	840.97	Joback Method
cpg	415.40	J/molxK	878.19	Joback Method
dvisc	0.0009297	Paxs	428.16	Joback Method
dvisc	0.0006257	Paxs	465.94	Joback Method

dvisc	0.0004469	Paxs	503.72	Joback Method
dvisc	0.0003345	Paxs	541.50	Joback Method
dvisc	0.0002601	Paxs	579.29	Joback Method
dvisc	0.0002085	Paxs	617.07	Joback Method
dvisc	0.0001715	Paxs	654.85	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C20330909&Units=SI

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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