

Isophthalic acid, 2-chloro-5-methylphenyl octyl ester

Inchi:	InChI=1S/C23H27ClO4/c1-3-4-5-6-7-8-14-27-22(25)18-10-9-11-19(16-18)23(26)28-21-15
InchiKey:	FAHZFNBZJIHRJB-UHFFFAOYSA-N
Formula:	C23H27ClO4
SMILES:	CCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2Cl)c1
Mol. weight [g/mol]:	402.91

Physical Properties

Property code	Value	Unit	Source
gf	-141.06	kJ/mol	Joback Method
hf	-584.74	kJ/mol	Joback Method
hfus	52.01	kJ/mol	Joback Method
hvap	96.03	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.385		Crippen Method
mvol	314.530	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	3062.00		NIST Webbook
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tb	983.95	K	Joback Method
tc	1212.54	K	Joback Method
tf	613.61	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.51	J/molxK	983.95	Joback Method
cpg	1027.76	J/molxK	1174.44	Joback Method
cpg	1020.34	J/molxK	1136.34	Joback Method
cpg	1011.65	J/molxK	1098.25	Joback Method
cpg	1001.64	J/molxK	1060.15	Joback Method
cpg	990.27	J/molxK	1022.05	Joback Method
cpg	1033.93	J/molxK	1212.54	Joback Method
dvisc	0.0000329	Paxs	983.95	Joback Method

dvisc	0.0000411	Paxs	922.23	Joback Method
dvisc	0.0000531	Paxs	860.50	Joback Method
dvisc	0.0000714	Paxs	798.78	Joback Method
dvisc	0.0001009	Paxs	737.06	Joback Method
dvisc	0.0001519	Paxs	675.33	Joback Method
dvisc	0.0002483	Paxs	613.61	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=U356570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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