

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

Inchi:	InChI=1S/C25H31ClO4/c1-3-4-5-6-7-8-9-10-16-29-24(27)20-12-11-13-21(18-20)25(28)30
InchiKey:	KXJSBXLCSJWDJT-UHFFFAOYSA-N
Formula:	C25H31ClO4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)c(C)c2)c1
Mol. weight [g/mol]:	430.96

Physical Properties

Property code	Value	Unit	Source
gf	-124.22	kJ/mol	Joback Method
hf	-626.02	kJ/mol	Joback Method
hfus	57.19	kJ/mol	Joback Method
hvap	100.48	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	7.165		Crippen Method
mvol	342.710	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	3429.00		NIST Webbook
rinpol	3429.00		NIST Webbook
tb	1029.71	K	Joback Method
tc	1262.57	K	Joback Method
tf	636.15	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.12	J/molxK	1029.71	Joback Method
cpg	1146.90	J/molxK	1223.76	Joback Method
cpg	1139.73	J/molxK	1184.95	Joback Method
cpg	1131.23	J/molxK	1146.14	Joback Method
cpg	1121.32	J/molxK	1107.33	Joback Method
cpg	1109.97	J/molxK	1068.52	Joback Method
cpg	1152.76	J/molxK	1262.57	Joback Method
dvisc	0.0000244	Paxs	1029.71	Joback Method

dvisc	0.0000307	Paxs	964.12	Joback Method
dvisc	0.0000400	Paxs	898.52	Joback Method
dvisc	0.0000543	Paxs	832.93	Joback Method
dvisc	0.0000777	Paxs	767.34	Joback Method
dvisc	0.0001188	Paxs	701.74	Joback Method
dvisc	0.0001982	Paxs	636.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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