

Isophthalic acid, 4-chloro-2-methylphenyl isoheptyl ester

Inchi:	InChI=1S/C21H23ClO4/c1-14(2)6-5-11-25-20(23)16-7-4-8-17(13-16)21(24)26-19-10-9-18
InchiKey:	IYOIXDLVMYCKMW-UHFFFAOYSA-N
Formula:	C21H23ClO4
SMILES:	Cc1cc(Cl)ccc1OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	374.86

Physical Properties

Property code	Value	Unit	Source
gf	-160.34	kJ/mol	Joback Method
hf	-548.74	kJ/mol	Joback Method
hfus	43.31	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.461		Crippen Method
mvol	286.350	ml/mol	McGowan Method
pc	1533.06	kPa	Joback Method
rinpol	2883.00		NIST Webbook
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tb	937.75	K	Joback Method
tc	1168.01	K	Joback Method
tf	576.07	K	Joback Method
vc	1.087	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.43	J/molxK	937.75	Joback Method
cpg	910.82	J/molxK	1129.64	Joback Method
cpg	903.35	J/molxK	1091.26	Joback Method
cpg	894.60	J/molxK	1052.88	Joback Method
cpg	884.55	J/molxK	1014.50	Joback Method
cpg	873.18	J/molxK	976.13	Joback Method
cpg	917.06	J/molxK	1168.01	Joback Method
dvisc	0.0000400	Paxs	937.75	Joback Method

dvisc	0.0000504	Paxs	877.47	Joback Method
dvisc	0.0000656	Paxs	817.19	Joback Method
dvisc	0.0000891	Paxs	756.91	Joback Method
dvisc	0.0001277	Paxs	696.63	Joback Method
dvisc	0.0001959	Paxs	636.35	Joback Method
dvisc	0.0003287	Paxs	576.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344646&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

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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