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

Inchi: InChI=1S/C22H25ClO4/c1-3-4-5-6-7-13-26-21(24)17-9-8-10-18(15-17)22(25)27-20-14-16

InchiKey: AFOLSICZMGJBHO-UHFFFAOYSA-N

Formula: C22H25ClO4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2Cl)c1

Mol. weight [g/mol]: 388.88

Physical Properties

Property code	Value	Unit	Source
gf	-149.48	kJ/mol	Joback Method
hf	-564.10	kJ/mol	Joback Method
hfus	49.42	kJ/mol	Joback Method
hvap	93.80	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.995		Crippen Method
mcvol	300.440	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2951.00		NIST Webbook
rinpol	2951.00		NIST Webbook
tb	961.07	K	Joback Method
tc	1188.91	K	Joback Method
tf	602.34	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.44	J/mol×K	961.07	Joback Method
cpg	931.16	J/mol×K	999.04	Joback Method
cpg	942.53	J/mol×K	1037.02	Joback Method
cpg	952.57	J/mol×K	1074.99	Joback Method
cpg	961.32	J/mol×K	1112.96	Joback Method
cpg	968.82	J/mol×K	1150.94	Joback Method
cpg	975.10	J/mol×K	1188.91	Joback Method
dvisc	0.0002765	Pa×s	602.34	Joback Method

dvisc	0.0001711	Pa×s	662.13	Joback Method
dvisc	0.0001146	Pa×s	721.92	Joback Method
dvisc	0.0000816	Pa×s	781.71	Joback Method
dvisc	0.0000610	Pa×s	841.49	Joback Method
dvisc	0.0000474	Pa×s	901.28	Joback Method
dvisc	0.0000380	Pa×s	961.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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