Isophthalic acid, 4-chlorophenyl octyl ester

Inchi: InChI=1S/C22H25ClO4/c1-2-3-4-5-6-7-15-26-21(24)17-9-8-10-18(16-17)22(25)27-20-13-
InchiKey: JNBIFKODUGXLPM-UHFFFAOYSA-N
Formula: C22H25ClO4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 388.88

Physical Properties

Property code	Value	Unit	Source
gf	-139.85	kJ/mol	Joback Method
hf	-552.63	kJ/mol	Joback Method
hfus	49.81	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.077		Crippen Method
mcvol	300.440	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	3115.00		NIST Webbook
rinpol	3115.00		NIST Webbook
tb	956.09	K	Joback Method
tc	1183.10	K	Joback Method
tf	589.82	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.72	J/mol×K	956.09	Joback Method
cpg	932.57	J/mol×K	993.93	Joback Method
cpg	944.09	J/mol×K	1031.76	Joback Method
cpg	954.31	J/mol×K	1069.60	Joback Method
cpg	963.29	J/mol×K	1107.43	Joback Method
cpg	971.07	J/mol×K	1145.27	Joback Method
cpg	977.69	J/mol×K	1183.10	Joback Method
dvisc	0.0003074	Pa×s	589.82	Joback Method

dvisc	0.0001832	Pa×s	650.87	Joback Method
dvisc	0.0001193	Pa×s	711.91	Joback Method
dvisc	0.0000832	Pa×s	772.95	Joback Method
dvisc	0.0000611	Pa×s	834.00	Joback Method
dvisc	0.0000468	Pa×s	895.04	Joback Method
dvisc	0.0000371	Pa×s	956.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344583&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
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