Isophthalic acid, decyl 2,5-dichlorophenyl ester

Inchi: InChI=1S/C24H28Cl2O4/c1-2-3-4-5-6-7-8-9-15-29-23(27)18-11-10-12-19(16-18)24(28)30

InchiKey: YCLDPPJSHQMWRM-UHFFFAOYSA-N

Formula: C24H28Cl2O4

SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)ccc2Cl)c1

Mol. weight [g/mol]: 451.38

Physical Properties

Property code	Value	Unit	Source
gf	-144.57	kJ/mol	Joback Method
hf	-621.12	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	102.64	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.510		Crippen Method
mcvol	340.860	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	3428.00		NIST Webbook
rinpol	3428.00		NIST Webbook
tb	1044.26	K	Joback Method
tc	1280.83	K	Joback Method
tf	654.80	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.56	J/mol×K	1044.26	Joback Method
cpg	1069.02	J/mol×K	1083.69	Joback Method
cpg	1079.02	J/mol×K	1123.12	Joback Method
cpg	1087.63	J/mol×K	1162.54	Joback Method
cpg	1094.89	J/mol×K	1201.97	Joback Method
cpg	1100.85	J/mol×K	1241.40	Joback Method
cpg	1105.58	J/mol×K	1280.83	Joback Method
dvisc	0.0001817	Pa×s	654.80	Joback Method

dvisc	0.0001113	Pa×s	719.71	Joback Method
dvisc	0.0000739	Pa×s	784.62	Joback Method
dvisc	0.0000522	Pa×s	849.53	Joback Method
dvisc	0.0000388	Pa×s	914.44	Joback Method
dvisc	0.0000299	Pa×s	979.35	Joback Method
dvisc	0.0000239	Pa×s	1044.26	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=U344706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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