

Isophthalic acid, 4-chlorophenyl dodecyl ester

Inchi: InChI=1S/C26H33ClO4/c1-2-3-4-5-6-7-8-9-10-11-19-30-25(28)21-13-12-14-22(20-21)26
InchiKey: IBYBWSHZDQBAQT-UHFFFAOYSA-N
Formula: C26H33ClO4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 444.99

Physical Properties

Property code	Value	Unit	Source
gf	-106.17	kJ/mol	Joback Method
hf	-635.19	kJ/mol	Joback Method
hfus	60.17	kJ/mol	Joback Method
hvap	102.04	kJ/mol	Joback Method
log10ws	-9.09		Crippen Method
logp	7.637		Crippen Method
mvol	356.800	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	3542.00		NIST Webbook
tb	1047.61	K	Joback Method
tc	1283.06	K	Joback Method
tf	634.90	K	Joback Method
vc	1.373	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.89	J/molxK	1047.61	Joback Method
cpg	1209.96	J/molxK	1243.81	Joback Method
cpg	1202.51	J/molxK	1204.57	Joback Method
cpg	1193.74	J/molxK	1165.33	Joback Method
cpg	1183.59	J/molxK	1126.09	Joback Method
cpg	1172.00	J/molxK	1086.85	Joback Method
cpg	1216.16	J/molxK	1283.06	Joback Method
dvisc	0.0000204	Paxs	1047.61	Joback Method
dvisc	0.0000260	Paxs	978.82	Joback Method

dvisc	0.0000344	Paxs	910.04	Joback Method
dvisc	0.0000477	Paxs	841.25	Joback Method
dvisc	0.0000701	Paxs	772.47	Joback Method
dvisc	0.0001110	Paxs	703.68	Joback Method
dvisc	0.0001941	Paxs	634.90	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344586&Units=SI

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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