

Isophthalic acid, 4-chlorophenyl ethyl ester

Inchi: InChI=1S/C16H13ClO4/c1-2-20-15(18)11-4-3-5-12(10-11)16(19)21-14-8-6-13(17)7-9-14/
InchiKey: QZPCJKASLCLXHE-UHFFFAOYSA-N
Formula: C16H13ClO4
SMILES: CCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 304.73

Physical Properties

Property code	Value	Unit	Source
gf	-190.37	kJ/mol	Joback Method
hf	-428.79	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.736		Crippen Method
mcvol	215.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	818.81	K	Joback Method
tc	1057.73	K	Joback Method
tf	522.20	K	Joback Method
vc	0.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.61	J/molxK	818.81	Joback Method
cpg	591.66	J/molxK	858.63	Joback Method
cpg	602.52	J/molxK	898.45	Joback Method
cpg	612.21	J/molxK	938.27	Joback Method
cpg	620.74	J/molxK	978.09	Joback Method
cpg	628.16	J/molxK	1017.91	Joback Method
cpg	634.47	J/molxK	1057.73	Joback Method
dvisc	0.0005504	Paxs	522.20	Joback Method

dvisc	0.0003526	Paxs	571.63	Joback Method
dvisc	0.0002425	Paxs	621.07	Joback Method
dvisc	0.0001762	Paxs	670.50	Joback Method
dvisc	0.0001338	Paxs	719.94	Joback Method
dvisc	0.0001052	Paxs	769.38	Joback Method
dvisc	0.0000852	Paxs	818.81	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344575&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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