

Terephthalic acid, 2-chloropropyl isobutyl ester

Inchi:	InChI=1S/C15H19ClO4/c1-10(2)8-19-14(17)12-4-6-13(7-5-12)15(18)20-9-11(3)16/h4-7,1
InchiKey:	OXIFJUVHBKBBNV-UHFFFAOYSA-N
Formula:	C15H19ClO4
SMILES:	CC(C)COC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]:	298.76

Physical Properties

Property code	Value	Unit	Source
gf	-306.45	kJ/mol	Joback Method
hf	-643.77	kJ/mol	Joback Method
hfus	30.98	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.283		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinsol	2106.00		NIST Webbook
tb	763.39	K	Joback Method
tc	976.92	K	Joback Method
tf	441.99	K	Joback Method
vc	0.853	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.20	J/molxK	763.39	Joback Method
cpg	635.31	J/molxK	798.98	Joback Method
cpg	648.39	J/molxK	834.57	Joback Method
cpg	660.46	J/molxK	870.16	Joback Method
cpg	671.51	J/molxK	905.74	Joback Method
cpg	681.57	J/molxK	941.33	Joback Method
cpg	690.64	J/molxK	976.92	Joback Method
dvisc	0.0010379	Paxs	441.99	Joback Method
dvisc	0.0005378	Paxs	495.56	Joback Method

dvisc	0.0003168	Paxs	549.12	Joback Method
dvisc	0.0002050	Paxs	602.69	Joback Method
dvisc	0.0001424	Paxs	656.26	Joback Method
dvisc	0.0001046	Paxs	709.82	Joback Method
dvisc	0.0000802	Paxs	763.39	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=U356169&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
mccvol:	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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