

Terephthalic acid, butyl 2-chloropropyl ester

Inchi:	InChI=1S/C15H19ClO4/c1-3-4-9-19-14(17)12-5-7-13(8-6-12)15(18)20-10-11(2)16/h5-8,1
InchiKey:	DHOOPYDBBTWSFJ-UHFFFAOYSA-N
Formula:	C15H19ClO4
SMILES:	CCCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]:	298.76

Physical Properties

Property code	Value	Unit	Source
gf	-304.01	kJ/mol	Joback Method
hf	-638.49	kJ/mol	Joback Method
hfus	34.51	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.428		Crippen Method
mvol	225.570	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2155.00		NIST Webbook
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tb	763.83	K	Joback Method
tc	974.13	K	Joback Method
tf	456.99	K	Joback Method
vc	0.859	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.63	J/molxK	763.83	Joback Method
cpg	634.52	J/molxK	798.88	Joback Method
cpg	647.43	J/molxK	833.93	Joback Method
cpg	659.36	J/molxK	868.98	Joback Method
cpg	670.31	J/molxK	904.03	Joback Method
cpg	680.32	J/molxK	939.08	Joback Method
cpg	689.38	J/molxK	974.13	Joback Method
dvisc	0.0008947	Paxs	456.99	Joback Method

dvisc	0.0004991	Paxs	508.13	Joback Method
dvisc	0.0003097	Paxs	559.27	Joback Method
dvisc	0.0002082	Paxs	610.41	Joback Method
dvisc	0.0001489	Paxs	661.55	Joback Method
dvisc	0.0001117	Paxs	712.69	Joback Method
dvisc	0.0000870	Paxs	763.83	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=U356170&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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