

Terephthalic acid, 2,2-dichloroethyl pentyl ester

Inchi:	InChI=1S/C15H18Cl2O4/c1-2-3-4-9-20-14(18)11-5-7-12(8-6-11)15(19)21-10-13(16)17/h5
InchiKey:	SVHGCUIONYMSPI-UHFFFAOYSA-N
Formula:	C15H18Cl2O4
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	333.21

Physical Properties

Property code	Value	Unit	Source
gf	-315.94	kJ/mol	Joback Method
hf	-654.23	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.994		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	801.26	K	Joback Method
tc	1015.00	K	Joback Method
tf	486.91	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.29	J/molxK	801.26	Joback Method
cpg	658.03	J/molxK	836.88	Joback Method
cpg	669.76	J/molxK	872.51	Joback Method
cpg	680.50	J/molxK	908.13	Joback Method
cpg	690.27	J/molxK	943.76	Joback Method
cpg	699.08	J/molxK	979.38	Joback Method
cpg	706.94	J/molxK	1015.00	Joback Method
dvisc	0.0007403	Paxs	486.91	Joback Method

dvisc	0.0004216	Paxs	539.30	Joback Method
dvisc	0.0002653	Paxs	591.69	Joback Method
dvisc	0.0001800	Paxs	644.09	Joback Method
dvisc	0.0001294	Paxs	696.48	Joback Method
dvisc	0.0000975	Paxs	748.87	Joback Method
dvisc	0.0000762	Paxs	801.26	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=U356245&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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