Bis(2,2-dichloroethyl) phthalate

Other names: 1,2-Benzenedicarboxylic acid, bis(2,2-dichloroethyl) ester
Bis(2,2-dichloroethyl)-1,2-benzenedicarboxylate
Inchi: InChI=1S/C12H10Cl4O4/c13-9(14)5-19-11(17)7-3-1-2-4-8(7)12(18)20-6-10(15)16/h1-4,9
InchiKey: ARHOBCWTZNGLEI-UHFFFAOYSA-N
Formula: C12H10Cl4O4
SMILES: O=C(OCC(Cl)Cl)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 360.02

Physical Properties

Property code	Value	Unit	Source
gf	-367.50	kJ/mol	Joback Method
hf	-629.07	kJ/mol	Joback Method
hfus	35.80	kJ/mol	Joback Method
hvap	80.32	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.608		Crippen Method
mcvol	220.020	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	807.04	K	Joback Method
tc	1038.33	K	Joback Method
tf	497.94	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.04	J/mol×K	807.04	Joback Method
cpg	537.52	J/mol×K	845.59	Joback Method
cpg	546.04	J/mol×K	884.14	Joback Method
cpg	553.63	J/mol×K	922.69	Joback Method
cpg	560.28	J/mol×K	961.24	Joback Method
cpg	566.02	J/mol×K	999.79	Joback Method

cpg	570.86	J/mol×K	1038.33	Joback Method
dvisc	0.0007558	Pa×s	497.94	Joback Method
dvisc	0.0004362	Pa×s	549.46	Joback Method
dvisc	0.0002766	Pa×s	600.97	Joback Method
dvisc	0.0001885	Pa×s	652.49	Joback Method
dvisc	0.0001358	Pa×s	704.01	Joback Method
dvisc	0.0001024	Pa×s	755.52	Joback Method
dvisc	0.0000800	Pa×s	807.04	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=U373666&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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