

Terephthalic acid, butyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C14H16Cl2O4/c1-2-3-8-19-13(17)10-4-6-11(7-5-10)14(18)20-9-12(15)16/h4-7,
InchiKey:	BNJZLSJZNILXGC-UHFFFAOYSA-N
Formula:	C14H16Cl2O4
SMILES:	CCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	319.18

Physical Properties

Property code	Value	Unit	Source
gf	-324.36	kJ/mol	Joback Method
hf	-633.59	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	76.39	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.604		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinsol	2209.00		NIST Webbook
tb	778.38	K	Joback Method
tc	994.35	K	Joback Method
tf	475.64	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.88	J/molxK	778.38	Joback Method
cpg	603.29	J/molxK	814.37	Joback Method
cpg	614.73	J/molxK	850.37	Joback Method
cpg	625.21	J/molxK	886.36	Joback Method
cpg	634.74	J/molxK	922.36	Joback Method
cpg	643.35	J/molxK	958.35	Joback Method
cpg	651.03	J/molxK	994.35	Joback Method
dvisc	0.0008144	Paxs	475.64	Joback Method
dvisc	0.0004698	Paxs	526.10	Joback Method

dvisc	0.0002984	Paxs	576.55	Joback Method
dvisc	0.0002039	Paxs	627.01	Joback Method
dvisc	0.0001475	Paxs	677.47	Joback Method
dvisc	0.0001116	Paxs	727.92	Joback Method
dvisc	0.0000875	Paxs	778.38	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=U356244&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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