

Terephthalic acid, 2,2-dichloroethyl heptyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-2-3-4-5-6-11-22-16(20)13-7-9-14(10-8-13)17(21)23-12-15(18)
InchiKey:	ABGGPJXFOZFNSE-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-299.10	kJ/mol	Joback Method
hf	-695.51	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	83.07	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.774		Crippen Method
mvol	265.990	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2533.00		NIST Webbook
tb	847.02	K	Joback Method
tc	1058.12	K	Joback Method
tf	509.45	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.99	J/molxK	847.02	Joback Method
cpg	770.24	J/molxK	882.20	Joback Method
cpg	782.42	J/molxK	917.39	Joback Method
cpg	793.55	J/molxK	952.57	Joback Method
cpg	803.65	J/molxK	987.75	Joback Method
cpg	812.74	J/molxK	1022.93	Joback Method
cpg	820.83	J/molxK	1058.12	Joback Method
dvisc	0.0006037	Paxs	509.45	Joback Method
dvisc	0.0003354	Paxs	565.71	Joback Method

dvisc	0.0002073	Paxs	621.97	Joback Method
dvisc	0.0001387	Paxs	678.24	Joback Method
dvisc	0.0000988	Paxs	734.50	Joback Method
dvisc	0.0000738	Paxs	790.76	Joback Method
dvisc	0.0000573	Paxs	847.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356247&Units=SI
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

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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