

Terephthalic acid, 2,2-dichloroethyl octyl ester

Inchi:	InChI=1S/C18H24Cl2O4/c1-2-3-4-5-6-7-12-23-17(21)14-8-10-15(11-9-14)18(22)24-13-16
InchiKey:	WIIRDTTWUSYVJF-UHFFFAOYSA-N
Formula:	C18H24Cl2O4
SMILES:	CCCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	375.29

Physical Properties

Property code	Value	Unit	Source
gf	-290.68	kJ/mol	Joback Method
hf	-716.15	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.164		Crippen Method
mcvol	280.080	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinsol	2638.00		NIST Webbook
tb	869.90	K	Joback Method
tc	1080.66	K	Joback Method
tf	520.72	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.13	J/molxK	869.90	Joback Method
cpg	870.60	J/molxK	1045.54	Joback Method
cpg	861.43	J/molxK	1010.41	Joback Method
cpg	851.23	J/molxK	975.28	Joback Method
cpg	839.96	J/molxK	940.15	Joback Method
cpg	827.60	J/molxK	905.03	Joback Method
cpg	878.75	J/molxK	1080.66	Joback Method
dvisc	0.0000495	Paxs	869.90	Joback Method
dvisc	0.0000639	Paxs	811.70	Joback Method

dvisc	0.0000859	Paxs	753.51	Joback Method
dvisc	0.0001213	Paxs	695.31	Joback Method
dvisc	0.0001824	Paxs	637.11	Joback Method
dvisc	0.0002976	Paxs	578.92	Joback Method
dvisc	0.0005419	Paxs	520.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356248&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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