

Terephthalic acid, decyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C20H28Cl2O4/c1-2-3-4-5-6-7-8-9-14-25-19(23)16-10-12-17(13-11-16)20(24)2
InchiKey:	GOZUFXQUSQRGOK-UHFFFAOYSA-N
Formula:	C20H28Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1ccc(C(=O)OCC(Cl)Cl)cc1
Mol. weight [g/mol]:	403.34

Physical Properties

Property code	Value	Unit	Source
gf	-273.84	kJ/mol	Joback Method
hf	-757.43	kJ/mol	Joback Method
hfus	51.65	kJ/mol	Joback Method
hvap	89.75	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.945		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinqol	2841.00		NIST Webbook
tb	915.66	K	Joback Method
tc	1127.99	K	Joback Method
tf	543.26	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.66	J/molxK	915.66	Joback Method
cpg	944.51	J/molxK	951.05	Joback Method
cpg	957.16	J/molxK	986.44	Joback Method
cpg	968.65	J/molxK	1021.82	Joback Method
cpg	978.99	J/molxK	1057.21	Joback Method
cpg	988.23	J/molxK	1092.60	Joback Method
cpg	996.40	J/molxK	1127.99	Joback Method
dvisc	0.0004320	Paxs	543.26	Joback Method
dvisc	0.0002321	Paxs	605.33	Joback Method

dvisc	0.0001399	Paxs	667.39	Joback Method
dvisc	0.0000920	Paxs	729.46	Joback Method
dvisc	0.0000645	Paxs	791.53	Joback Method
dvisc	0.0000477	Paxs	853.59	Joback Method
dvisc	0.0000367	Paxs	915.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356249&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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