Phthalic acid, decyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C20H28Cl2O4/c1-2-3-4-5-6-7-8-11-14-25-19(23)16-12-9-10-13-17(16)20(24)26
InchiKey: FXZIVYLBVMMJMI-UHFFFAOYSA-N
Formula: C20H28Cl2O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
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
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	915.66	K	Joback Method
tc	1127.99	K	Joback Method
tf	543.26	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.66	J/mol×K	915.66	Joback Method
cpg	944.51	J/mol×K	951.05	Joback Method
cpg	957.16	J/mol×K	986.44	Joback Method
cpg	968.65	J/mol×K	1021.82	Joback Method
cpg	978.99	J/mol×K	1057.21	Joback Method
cpg	988.23	J/mol×K	1092.60	Joback Method
cpg	996.40	J/mol×K	1127.99	Joback Method
dvisc	0.0004320	Pa×s	543.26	Joback Method

dvisc	0.0002321	Pa×s	605.33	Joback Method
dvisc	0.0001399	Pa×s	667.39	Joback Method
dvisc	0.0000920	Pa×s	729.46	Joback Method
dvisc	0.0000645	Pa×s	791.53	Joback Method
dvisc	0.0000477	Pa×s	853.59	Joback Method
dvisc	0.0000367	Pa×s	915.66	Joback Method

Sources

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=U356931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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