

Phthalic acid, 2,5-dichlorophenyl propyl ester

Inchi:	InChI=1S/C17H14Cl2O4/c1-2-9-22-16(20)12-5-3-4-6-13(12)17(21)23-15-10-11(18)7-8-14
InchiKey:	RNRGDFNTNQCGBK-UHFFFAOYSA-N
Formula:	C17H14Cl2O4
SMILES:	CCCOC(=O)c1ccccc1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	353.20

Physical Properties

Property code	Value	Unit	Source
gf	-203.51	kJ/mol	Joback Method
hf	-476.64	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.779		Crippen Method
mvol	242.230	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2477.00		NIST Webbook
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tb	884.10	K	Joback Method
tc	1122.62	K	Joback Method
tf	575.91	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.59	J/molxK	884.10	Joback Method
cpg	695.80	J/molxK	1082.87	Joback Method
cpg	689.70	J/molxK	1043.11	Joback Method
cpg	682.45	J/molxK	1003.36	Joback Method
cpg	674.03	J/molxK	963.61	Joback Method
cpg	664.42	J/molxK	923.85	Joback Method
cpg	700.78	J/molxK	1122.62	Joback Method
dvisc	0.0000663	Paxs	884.10	Joback Method

dvisc	0.0000811	Paxs	832.73	Joback Method
dvisc	0.0001020	Paxs	781.37	Joback Method
dvisc	0.0001325	Paxs	730.00	Joback Method
dvisc	0.0001791	Paxs	678.64	Joback Method
dvisc	0.0002542	Paxs	627.28	Joback Method
dvisc	0.0003841	Paxs	575.91	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=U356377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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