

Phthalic acid, 2,2-dichloroethyl nonyl ester

Inchi:	InChI=1S/C19H26Cl2O4/c1-2-3-4-5-6-7-10-13-24-18(22)15-11-8-9-12-16(15)19(23)25-14
InchiKey:	UGNGSARBXWZPHB-UHFFFAOYSA-N
Formula:	C19H26Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	389.31

Physical Properties

Property code	Value	Unit	Source
gf	-282.26	kJ/mol	Joback Method
hf	-736.79	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	87.52	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.554		Crippen Method
mvol	294.170	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	892.78	K	Joback Method
tc	1103.94	K	Joback Method
tf	531.99	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.04	J/mol×K	892.78	Joback Method
cpg	885.71	J/mol×K	927.97	Joback Method
cpg	898.22	J/mol×K	963.17	Joback Method
cpg	909.60	J/mol×K	998.36	Joback Method
cpg	919.89	J/mol×K	1033.55	Joback Method
cpg	929.11	J/mol×K	1068.74	Joback Method
cpg	937.29	J/mol×K	1103.94	Joback Method
dvisc	0.0004847	Paxs	531.99	Joback Method

dvisc	0.0002632	Paxs	592.12	Joback Method
dvisc	0.0001600	Paxs	652.25	Joback Method
dvisc	0.0001057	Paxs	712.38	Joback Method
dvisc	0.0000746	Paxs	772.52	Joback Method
dvisc	0.0000553	Paxs	832.65	Joback Method
dvisc	0.0000427	Paxs	892.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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