

Phthalic acid, pentyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C21H24O5/c1-2-3-9-14-25-20(22)18-12-7-8-13-19(18)21(23)26-16-15-24-17-1
InchiKey:	BCECSOFEJUFHAV-UHFFFAOYSA-N
Formula:	C21H24O5
SMILES:	CCCCCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	356.41

Physical Properties

Property code	Value	Unit	Source
gf	-231.71	kJ/mol	Joback Method
hf	-637.00	kJ/mol	Joback Method
hfus	44.60	kJ/mol	Joback Method
hvap	88.28	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.269		Crippen Method
mvol	279.980	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	3078.00		NIST Webbook
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tb	913.22	K	Joback Method
tc	1135.44	K	Joback Method
tf	558.34	K	Joback Method
vc	1.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.73	J/molxK	913.22	Joback Method
cpg	880.24	J/molxK	950.26	Joback Method
cpg	892.35	J/molxK	987.29	Joback Method
cpg	903.09	J/molxK	1024.33	Joback Method
cpg	912.49	J/molxK	1061.37	Joback Method
cpg	920.56	J/molxK	1098.41	Joback Method
cpg	927.34	J/molxK	1135.44	Joback Method
dvisc	0.0003303	Paxs	558.34	Joback Method

dvisc	0.0001920	Paxs	617.49	Joback Method
dvisc	0.0001227	Paxs	676.63	Joback Method
dvisc	0.0000843	Paxs	735.78	Joback Method
dvisc	0.0000612	Paxs	794.93	Joback Method
dvisc	0.0000465	Paxs	854.07	Joback Method
dvisc	0.0000366	Paxs	913.22	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=U382481&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
mc_{vol}:	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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