

Phthalic acid, ethyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C18H18O5/c1-2-21-17(19)15-10-6-7-11-16(15)18(20)23-13-12-22-14-8-4-3-5-9
InchiKey:	GXXXPIOHYCMQNG-UHFFFAOYSA-N
Formula:	C18H18O5
SMILES:	CCOC(=O)c1ccccc1C(=O)OCCOc1ccccc1
Mol. weight [g/mol]:	314.33

Physical Properties

Property code	Value	Unit	Source
gf	-256.97	kJ/mol	Joback Method
hf	-575.08	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.099		Crippen Method
mvol	237.710	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2786.00		NIST Webbook
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tb	844.58	K	Joback Method
tc	1071.29	K	Joback Method
tf	524.53	K	Joback Method
vc	0.893	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.84	J/molxK	844.58	Joback Method
cpg	708.18	J/molxK	882.36	Joback Method
cpg	720.21	J/molxK	920.15	Joback Method
cpg	730.95	J/molxK	957.93	Joback Method
cpg	740.42	J/molxK	995.72	Joback Method
cpg	748.63	J/molxK	1033.50	Joback Method
cpg	755.59	J/molxK	1071.29	Joback Method
dvisc	0.0004449	Paxs	524.53	Joback Method

dvisc	0.0002680	Paxs	577.87	Joback Method
dvisc	0.0001759	Paxs	631.21	Joback Method
dvisc	0.0001233	Paxs	684.55	Joback Method
dvisc	0.0000910	Paxs	737.90	Joback Method
dvisc	0.0000699	Paxs	791.24	Joback Method
dvisc	0.0000556	Paxs	844.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382477&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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