

Phthalic acid, ethyl pent-4-enyl ester

Inchi:	InChI=1S/C15H18O4/c1-3-5-8-11-19-15(17)13-10-7-6-9-12(13)14(16)18-4-2/h3,6-7,9-10
InchiKey:	BLAVCVRCTOSDLW-UHFFFAOYSA-N
Formula:	C15H18O4
SMILES:	C=CCCCOC(=O)c1cccc1C(=O)OCC
Mol. weight [g/mol]:	262.30

Physical Properties

Property code	Value	Unit	Source
gf	-201.80	kJ/mol	Joback Method
hf	-492.04	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.986		Crippen Method
mcvol	209.030	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1887.00		NIST Webbook
tb	723.52	K	Joback Method
tc	930.26	K	Joback Method
tf	440.31	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.26	J/molxK	723.52	Joback Method
cpg	583.49	J/molxK	757.98	Joback Method
cpg	596.78	J/molxK	792.43	Joback Method
cpg	609.17	J/molxK	826.89	Joback Method
cpg	620.66	J/molxK	861.35	Joback Method
cpg	631.28	J/molxK	895.80	Joback Method
cpg	641.02	J/molxK	930.26	Joback Method
dvisc	0.0009235	Paxs	440.31	Joback Method
dvisc	0.0005476	Paxs	487.51	Joback Method

dvisc	0.0003561	Paxs	534.71	Joback Method
dvisc	0.0002483	Paxs	581.91	Joback Method
dvisc	0.0001828	Paxs	629.12	Joback Method
dvisc	0.0001404	Paxs	676.32	Joback Method
dvisc	0.0001117	Paxs	723.52	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=U360462&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

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