

Phthalic acid, ethyl trans-hex-3-enyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H20O4/c1-3-5-6-9-12-20-16(18)14-11-8-7-10-13(14)15(17)19-4-2/h5-8,10-

WIMARXSQHUWBAH-AATRIKPKSA-N

C16H20O4

CCC=CCCOC(=O)c1ccccc1C(=O)OCC

276.33

Physical Properties

Property code	Value	Unit	Source
gf	-201.00	kJ/mol	Joback Method
hf	-520.89	kJ/mol	Joback Method
hfus	36.62	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.376		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	753.88	K	Joback Method
tc	961.93	K	Joback Method
tf	448.26	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.96	J/mol×K	753.88	Joback Method
cpg	638.55	J/mol×K	788.55	Joback Method
cpg	652.19	J/mol×K	823.23	Joback Method
cpg	664.89	J/mol×K	857.90	Joback Method
cpg	676.67	J/mol×K	892.58	Joback Method
cpg	687.57	J/mol×K	927.25	Joback Method
cpg	697.61	J/mol×K	961.93	Joback Method
dvisc	0.0007844	Pa×s	448.26	Joback Method

dvisc	0.0004428	Pa×s	499.20	Joback Method
dvisc	0.0002779	Pa×s	550.13	Joback Method
dvisc	0.0001887	Pa×s	601.07	Joback Method
dvisc	0.0001362	Pa×s	652.01	Joback Method
dvisc	0.0001030	Pa×s	702.94	Joback Method
dvisc	0.0000809	Pa×s	753.88	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=U360479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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