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

Inchi: 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-
InchiKey: WIMARXSQHUWBAH-WAYWQWQTSA-N
Formula: C16H20O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)OCC
Mol. weight [g/mol]: 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	1985.00		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=U360275&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