Dipent-4-enyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, dipent-4-enyl ester
	Dipent-4-enyl-1,2-benzenedicarboxylate
	Phthalic acid, di(pent-4-enyl) ester
Inchi:	InChI=1S/C18H22O4/c1-3-5-9-13-21-17(19)15-11-7-8-12-16(15)18(20)22-14-10-6-4-2/h3
InchiKey:	CMNXQCDLELQIQH-UHFFFAOYSA-N
Formula:	C18H22O4
SMILES:	C=CCCCOC(=O)c1ccccc1C(=O)OCCCC=C
Mol. weight [g/mol]:	302.36
CAS:	176533-57-6

Physical Properties

Property code	Value	Unit	Source
gf	-88.70	kJ/mol	Joback Method
hf	-428.53	kJ/mol	Joback Method
hfus	39.04	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.933		Crippen Method
mcvol	247.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2145.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	788.84	K	Joback Method
tc	993.01	K	Joback Method
tf	472.36	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.01	J/mol×K	788.84	Joback Method
cpg	723.67	J/mol×K	822.87	Joback Method
cpg	737.33	J/mol×K	856.90	Joback Method
cpg	750.02	J/mol×K	890.92	Joback Method

cpg	761.76	J/mol×K	924.95	Joback Method
cpg	772.57	J/mol×K	958.98	Joback Method
cpg	782.49	J/mol×K	993.01	Joback Method
dvisc	0.0007381	Pa×s	472.36	Joback Method
dvisc	0.0004252	Pa×s	525.11	Joback Method
dvisc	0.0002709	Pa×s	577.85	Joback Method
dvisc	0.0001861	Pa×s	630.60	Joback Method
dvisc	0.0001355	Pa×s	683.35	Joback Method
dvisc	0.0001032	Pa×s	736.09	Joback Method
dvisc	0.0000815	Pa×s	788.84	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=C176533576&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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