

Isophthalic acid, di(pent-4-enyl) ester

Inchi:	InChI=1S/C18H22O4/c1-3-5-7-12-21-17(19)15-10-9-11-16(14-15)18(20)22-13-8-6-4-2/h3
InchiKey:	NYNZBEXGNHUGPM-UHFFFAOYSA-N
Formula:	C18H22O4
SMILES:	C=CCCCOC(=O)c1cccc(C(=O)OCCCC=C)c1
Mol. weight [g/mol]:	302.36

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
mvol	247.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2241.00		NIST Webbook
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tb	788.84	K	Joback Method
tc	993.01	K	Joback Method
tf	472.36	K	Joback Method
vc	0.946	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.01	J/molxK	788.84	Joback Method
cpg	772.57	J/molxK	958.98	Joback Method
cpg	761.76	J/molxK	924.95	Joback Method
cpg	750.02	J/molxK	890.92	Joback Method
cpg	737.33	J/molxK	856.90	Joback Method
cpg	723.67	J/molxK	822.87	Joback Method
cpg	782.49	J/molxK	993.01	Joback Method
dvisc	0.0000815	Paxs	788.84	Joback Method

dvisc	0.0001032	Paxs	736.09	Joback Method
dvisc	0.0001355	Paxs	683.35	Joback Method
dvisc	0.0001861	Paxs	630.60	Joback Method
dvisc	0.0002709	Paxs	577.85	Joback Method
dvisc	0.0004252	Paxs	525.11	Joback Method
dvisc	0.0007381	Paxs	472.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356727&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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