

Isophthalic acid, cis-hex-3-enyl pentyl ester

Inchi:	InChI=1S/C19H26O4/c1-3-5-7-9-14-23-19(21)17-12-10-11-16(15-17)18(20)22-13-8-6-4-2
InchiKey:	QQBIVNHSISUJMO-ALCCZGGFSA-N
Formula:	C19H26O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-175.74	kJ/mol	Joback Method
hf	-582.81	kJ/mol	Joback Method
hfus	44.39	kJ/mol	Joback Method
hvap	79.10	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.547		Crippen Method
mcvol	265.390	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2348.00		NIST Webbook
tb	822.52	K	Joback Method
tc	1026.70	K	Joback Method
tf	482.07	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.06	J/molxK	822.52	Joback Method
cpg	808.50	J/molxK	856.55	Joback Method
cpg	822.88	J/molxK	890.58	Joback Method
cpg	836.26	J/molxK	924.61	Joback Method
cpg	848.65	J/molxK	958.64	Joback Method
cpg	860.10	J/molxK	992.67	Joback Method
cpg	870.63	J/molxK	1026.70	Joback Method
dvisc	0.0006034	Paxs	482.07	Joback Method
dvisc	0.0003277	Paxs	538.81	Joback Method

dvisc	0.0001999	Paxs	595.55	Joback Method
dvisc	0.0001329	Paxs	652.30	Joback Method
dvisc	0.0000944	Paxs	709.04	Joback Method
dvisc	0.0000705	Paxs	765.78	Joback Method
dvisc	0.0000548	Paxs	822.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356700&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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