

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

Inchi:	InChI=1S/C17H22O4/c1-3-5-6-7-12-21-17(19)15-10-8-9-14(13-15)16(18)20-11-4-2/h5-6,
InchiKey:	FOBIQWNQQYRDHL-WAYWQWQTSA-N
Formula:	C17H22O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCC)c1
Mol. weight [g/mol]:	290.35

Physical Properties

Property code	Value	Unit	Source
gf	-192.58	kJ/mol	Joback Method
hf	-541.53	kJ/mol	Joback Method
hfus	39.21	kJ/mol	Joback Method
hvap	74.64	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.766		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinsol	2153.00		NIST Webbook
tb	776.76	K	Joback Method
tc	982.95	K	Joback Method
tf	459.53	K	Joback Method
vc	0.907	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.33	J/molxK	776.76	Joback Method
cpg	694.24	J/molxK	811.12	Joback Method
cpg	708.16	J/molxK	845.49	Joback Method
cpg	721.12	J/molxK	879.85	Joback Method
cpg	733.15	J/molxK	914.22	Joback Method
cpg	744.26	J/molxK	948.58	Joback Method
cpg	754.50	J/molxK	982.95	Joback Method
dvisc	0.0007226	Paxs	459.53	Joback Method
dvisc	0.0004025	Paxs	512.40	Joback Method

dvisc	0.0002501	Paxs	565.27	Joback Method
dvisc	0.0001686	Paxs	618.14	Joback Method
dvisc	0.0001210	Paxs	671.02	Joback Method
dvisc	0.0000911	Paxs	723.89	Joback Method
dvisc	0.0000713	Paxs	776.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356697&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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