

Phthalic acid, hexyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C20H28O4/c1-3-5-7-11-15-23-19(21)17-13-9-10-14-18(17)20(22)24-16-12-8-6
InchiKey:	BNURUOWZODZXS-RFNORWQNLSA-N
Formula:	C20H28O4
SMILES:	CCC=CCCOC(=O)c1cccc1C(=O)OCCCCC
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-167.32	kJ/mol	Joback Method
hf	-603.45	kJ/mol	Joback Method
hfus	46.98	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.937		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinsol	2312.00		NIST Webbook
tb	845.40	K	Joback Method
tc	1049.53	K	Joback Method
tf	493.34	K	Joback Method
vc	1.075	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.27	J/molxK	845.40	Joback Method
cpg	919.19	J/molxK	1015.50	Joback Method
cpg	907.62	J/molxK	981.48	Joback Method
cpg	895.08	J/molxK	947.46	Joback Method
cpg	881.53	J/molxK	913.44	Joback Method
cpg	866.94	J/molxK	879.42	Joback Method
cpg	929.83	J/molxK	1049.53	Joback Method
dvisc	0.0000478	Paxs	845.40	Joback Method
dvisc	0.0000617	Paxs	786.72	Joback Method

dvisc	0.0000829	Paxs	728.05	Joback Method
dvisc	0.0001174	Paxs	669.37	Joback Method
dvisc	0.0001777	Paxs	610.69	Joback Method
dvisc	0.0002938	Paxs	552.02	Joback Method
dvisc	0.0005474	Paxs	493.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360484&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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