

Isophthalic acid, hexadecyl hexyl ester

Inchi:	InChI=1S/C30H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-25-34-30(32)28-23-21-
InchiKey:	ZYLOCUFAAXNDTK-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCCCC)c1
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	-163.34	kJ/mol	Joback Method
hf	-927.07	kJ/mol	Joback Method
hfus	72.68	kJ/mol	Joback Method
hvap	103.62	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.062		Crippen Method
mvol	424.680	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpol	3600.00		NIST Webbook
rinpol	3600.00		NIST Webbook
tb	1070.04	K	Joback Method
tc	1324.57	K	Joback Method
tf	611.12	K	Joback Method
vc	1.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.84	J/molxK	1070.04	Joback Method
cpg	1515.88	J/molxK	1112.46	Joback Method
cpg	1532.83	J/molxK	1154.88	Joback Method
cpg	1547.78	J/molxK	1197.31	Joback Method
cpg	1560.83	J/molxK	1239.73	Joback Method
cpg	1572.09	J/molxK	1282.15	Joback Method
cpg	1581.64	J/molxK	1324.57	Joback Method
dvisc	0.0001828	Paxs	611.12	Joback Method

dvisc	0.0000907	Paxs	687.61	Joback Method
dvisc	0.0000517	Paxs	764.09	Joback Method
dvisc	0.0000327	Paxs	840.58	Joback Method
dvisc	0.0000223	Paxs	917.07	Joback Method
dvisc	0.0000161	Paxs	993.55	Joback Method
dvisc	0.0000122	Paxs	1070.04	Joback Method

Sources

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=U344715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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