

Isophthalic acid, hexadecyl 3-methylpentyl ester

Inchi:	InChI=1S/C30H50O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-23-33-29(31)27-20-19-2
InchiKey:	VMKUUXGGKHMCRH-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCC(C)CC)c1
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	-165.78	kJ/mol	Joback Method
hf	-932.35	kJ/mol	Joback Method
hfus	69.16	kJ/mol	Joback Method
hvap	103.24	kJ/mol	Joback Method
log10ws	-10.09		Crippen Method
logp	8.918		Crippen Method
mvol	424.680	ml/mol	McGowan Method
pc	737.62	kPa	Joback Method
rinpol	3452.00		NIST Webbook
tb	1069.60	K	Joback Method
tc	1321.85	K	Joback Method
tf	596.12	K	Joback Method
vc	1.649	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.00	J/molxK	1069.60	Joback Method
cpg	1571.11	J/molxK	1279.81	Joback Method
cpg	1560.06	J/molxK	1237.77	Joback Method
cpg	1547.22	J/molxK	1195.73	Joback Method
cpg	1532.50	J/molxK	1153.68	Joback Method
cpg	1515.79	J/molxK	1111.64	Joback Method
cpg	1580.48	J/molxK	1321.85	Joback Method
dvisc	0.0000111	Paxs	1069.60	Joback Method
dvisc	0.0000148	Paxs	990.69	Joback Method

dvisc	0.0000208	Paxs	911.77	Joback Method
dvisc	0.0000312	Paxs	832.86	Joback Method
dvisc	0.0000509	Paxs	753.95	Joback Method
dvisc	0.0000931	Paxs	675.03	Joback Method
dvisc	0.0001997	Paxs	596.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356160&Units=SI

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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