

Terephthalic acid, hexadecyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C30H50O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-33-29(31)27-19-21-2
InchiKey:	JCMWFLHXNKMEFA-UHFFFAOYSA-N
Formula:	C30H50O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CC(C)C)cc1
Mol. weight [g/mol]:	474.72

Physical Properties

Property code	Value	Unit	Source
gf	-168.22	kJ/mol	Joback Method
hf	-937.63	kJ/mol	Joback Method
hfus	65.64	kJ/mol	Joback Method
hvap	102.85	kJ/mol	Joback Method
log10ws	-10.20		Crippen Method
logp	8.916		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	740.84	kPa	Joback Method
rinpol	3359.00		NIST Webbook
tb	1069.16	K	Joback Method
tc	1319.32	K	Joback Method
tf	581.12	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1497.17	J/molxK	1069.16	Joback Method
cpg	1570.20	J/molxK	1277.62	Joback Method
cpg	1559.34	J/molxK	1235.93	Joback Method
cpg	1546.71	J/molxK	1194.24	Joback Method
cpg	1532.20	J/molxK	1152.55	Joback Method
cpg	1515.72	J/molxK	1110.85	Joback Method
cpg	1579.37	J/molxK	1319.32	Joback Method
dvisc	0.0000101	Paxs	1069.16	Joback Method
dvisc	0.0000136	Paxs	987.82	Joback Method

dvisc	0.0000195	Paxs	906.48	Joback Method
dvisc	0.0000299	Paxs	825.14	Joback Method
dvisc	0.0000503	Paxs	743.80	Joback Method
dvisc	0.0000962	Paxs	662.46	Joback Method
dvisc	0.0002206	Paxs	581.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356267&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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