

Terephthalic acid, 5-methylhex-2-yl undecyl ester

Inchi:	InChI=1S/C26H42O4/c1-5-6-7-8-9-10-11-12-13-20-29-25(27)23-16-18-24(19-17-23)26(2
InchiKey:	CHCGXPDVPJWMRM-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-201.90	kJ/mol	Joback Method
hf	-855.07	kJ/mol	Joback Method
hfus	55.28	kJ/mol	Joback Method
hvap	93.94	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.356		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	923.86	kPa	Joback Method
rinpol	3367.00		NIST Webbook
rinpol	3367.00		NIST Webbook
tb	977.64	K	Joback Method
tc	1196.94	K	Joback Method
tf	536.04	K	Joback Method
vc	1.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.40	J/molxK	977.64	Joback Method
cpg	1261.82	J/molxK	1014.19	Joback Method
cpg	1277.68	J/molxK	1050.74	Joback Method
cpg	1292.02	J/molxK	1087.29	Joback Method
cpg	1304.91	J/molxK	1123.84	Joback Method
cpg	1316.39	J/molxK	1160.39	Joback Method
cpg	1326.50	J/molxK	1196.94	Joback Method
dvisc	0.0003771	Paxs	536.04	Joback Method

dvisc	0.0001694	Paxs	609.64	Joback Method
dvisc	0.0000904	Paxs	683.24	Joback Method
dvisc	0.0000545	Paxs	756.84	Joback Method
dvisc	0.0000360	Paxs	830.44	Joback Method
dvisc	0.0000254	Paxs	904.04	Joback Method
dvisc	0.0000189	Paxs	977.64	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=U383004&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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