Terephthalic acid, 2-decyl octyl ester

Inchi: InChI=1S/C26H42O4/c1-4-6-8-10-12-14-16-22(3)30-26(28)24-19-17-23(18-20-24)25(27)
InchiKey: AGUBEKOVELPQNC-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OC(C)CCCCCCCC)cc1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-199.46	kJ/mol	Joback Method
hf	-849.79	kJ/mol	Joback Method
hfus	58.80	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.500		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	2983.00		NIST Webbook
tb	978.08	K	Joback Method
tc	1197.65	K	Joback Method
tf	551.04	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.04	J/mol×K	978.08	Joback Method
cpg	1261.53	J/mol×K	1014.67	Joback Method
cpg	1277.47	J/mol×K	1051.27	Joback Method
cpg	1291.91	J/mol×K	1087.86	Joback Method
cpg	1304.90	J/mol×K	1124.46	Joback Method
cpg	1316.49	J/mol×K	1161.05	Joback Method
cpg	1326.73	J/mol×K	1197.65	Joback Method
dvisc	0.0003362	Pa×s	551.04	Joback Method
dvisc	0.0001620	Pa×s	622.21	Joback Method

dvisc	0.0000907	Pa×s	693.39	Joback Method
dvisc	0.0000566	Pa×s	764.56	Joback Method
dvisc	0.0000383	Pa×s	835.73	Joback Method
dvisc	0.0000275	Pa×s	906.91	Joback Method
dvisc	0.0000207	Pa×s	978.08	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U356217&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