Terephthalic acid, 3-methylpentyl pentyl ester

Inchi: InChI=1S/C19H28O4/c1-4-6-7-13-22-18(20)16-8-10-17(11-9-16)19(21)23-14-12-15(3)5-2
InchiKey: LYDGCSQDBIMJPJ-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCCCCOC(=O)c1ccc(C(=O)OCCC(C)CC)cc1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-258.40	kJ/mol	Joback Method
hf	-705.31	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.627		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	817.92	K	Joback Method
tc	1019.49	K	Joback Method
tf	472.15	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.59	J/mol×K	817.92	Joback Method
cpg	835.66	J/mol×K	851.51	Joback Method
cpg	850.61	J/mol×K	885.11	Joback Method
cpg	864.46	J/mol×K	918.70	Joback Method
cpg	877.24	J/mol×K	952.30	Joback Method
cpg	888.96	J/mol×K	985.89	Joback Method
cpg	899.64	J/mol×K	1019.49	Joback Method
dvisc	0.0007448	Pa×s	472.15	Joback Method

dvisc	0.0003857	Pa×s	529.78	Joback Method
dvisc	0.0002273	Pa×s	587.41	Joback Method
dvisc	0.0001472	Pa×s	645.03	Joback Method
dvisc	0.0001024	Pa×s	702.66	Joback Method
dvisc	0.0000752	Pa×s	760.29	Joback Method
dvisc	0.0000577	Pa×s	817.92	Joback Method

Sources

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=U356675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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