Terephthalic acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C24H38O4/c1-17(13-23(3,4)5)15-27-21(25)19-9-11-20(12-10-19)22(26)28-16-
InchiKey: WEMQQGBLMUDXIC-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CC(COC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1)CC(C)(C)C
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.06	kJ/mol	Joback Method
hf	-831.29	kJ/mol	Joback Method
hfus	35.27	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	6.145		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1067.97	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	925.42	K	Joback Method
tc	1141.24	K	Joback Method
tf	518.34	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.67	J/mol×K	925.42	Joback Method
cpg	1137.92	J/mol×K	961.39	Joback Method
cpg	1153.87	J/mol×K	997.36	Joback Method
cpg	1168.61	J/mol×K	1033.33	Joback Method
cpg	1182.22	J/mol×K	1069.30	Joback Method
cpg	1194.78	J/mol×K	1105.27	Joback Method
cpg	1206.37	J/mol×K	1141.24	Joback Method
dvisc	0.0003972	Pa×s	518.34	Joback Method

dvisc	0.0001683	Pa×s	586.19	Joback Method
dvisc	0.0000852	Pa×s	654.03	Joback Method
dvisc	0.0000490	Pa×s	721.88	Joback Method
dvisc	0.0000310	Pa×s	789.73	Joback Method
dvisc	0.0000211	Pa×s	857.57	Joback Method
dvisc	0.0000152	Pa×s	925.42	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=U416020&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