Terephthalic acid, pentyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C21H32O4/c1-6-7-8-13-24-19(22)17-9-11-18(12-10-17)20(23)25-15-16(2)14-2
InchiKey: YICIULMMOSOOSI-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCCCOC(=O)c1ccc(C(=O)OCC(C)CC(C)(C)C)cc1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-238.72	kJ/mol	Joback Method
hf	-755.34	kJ/mol	Joback Method
hfus	38.43	kJ/mol	Joback Method
hvap	81.91	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.263		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	860.45	K	Joback Method
tc	1067.71	K	Joback Method
tf	497.11	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.43	J/mol×K	860.45	Joback Method
cpg	955.02	J/mol×K	894.99	Joback Method
cpg	970.40	J/mol×K	929.54	Joback Method
cpg	984.62	J/mol×K	964.08	Joback Method
cpg	997.72	J/mol×K	998.62	Joback Method
cpg	1009.74	J/mol×K	1033.16	Joback Method
cpg	1020.73	J/mol×K	1067.71	Joback Method
dvisc	0.0005578	Pa×s	497.11	Joback Method

dvisc	0.0002722	Pa×s	557.67	Joback Method
dvisc	0.0001529	Pa×s	618.22	Joback Method
dvisc	0.0000952	Pa×s	678.78	Joback Method
dvisc	0.0000640	Pa×s	739.34	Joback Method
dvisc	0.0000457	Pa×s	799.89	Joback Method
dvisc	0.0000343	Pa×s	860.45	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=U416011&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