Terephthalic acid, di(5-methylhex-2-yl) ester

Inchi: InChI=1S/C22H34O4/c1-15(2)7-9-17(5)25-21(23)19-11-13-20(14-12-19)22(24)26-18(6)1
InchiKey: ZOQWJDQFSMAJRM-UHFFFAOYSA-N
Formula: C22H34O4
SMILES: CC(C)CCC(C)OC(=O)c1ccc(C(=O)OC(C)CCC(C)C)cc1
Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-240.46	kJ/mol	Joback Method
hf	-783.07	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.650		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2791.00		NIST Webbook
tb	885.24	K	Joback Method
tc	1093.62	K	Joback Method
tf	460.96	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.22	J/mol×K	885.24	Joback Method
cpg	1070.54	J/mol×K	1058.89	Joback Method
cpg	1058.83	J/mol×K	1024.16	Joback Method
cpg	1045.88	J/mol×K	989.43	Joback Method
cpg	1031.64	J/mol×K	954.70	Joback Method
cpg	1016.10	J/mol×K	919.97	Joback Method
cpg	1081.03	J/mol×K	1093.62	Joback Method
dvisc	0.0000288	Pa×s	885.24	Joback Method

dvisc	0.0000397	Pa×s	814.53	Joback Method
dvisc	0.0000580	Pa×s	743.81	Joback Method
dvisc	0.0000918	Pa×s	673.10	Joback Method
dvisc	0.0001619	Pa×s	602.39	Joback Method
dvisc	0.0003320	Pa×s	531.67	Joback Method
dvisc	0.0008484	Pa×s	460.96	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=U383008&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