Terephthalic acid, hexyl 6-methylhept-2-yl ester

Inchi: InChI=1S/C22H34O4/c1-5-6-7-8-16-25-21(23)19-12-14-20(15-13-19)22(24)26-18(4)11-9

InchiKey: YDJFLVXMHARBRO-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCCCCOC(=O)c1ccc(C(=O)OC(C)CCCC(C)C)cc1

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-235.58	kJ/mol	Joback Method
hf	-772.51	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.795		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2652.00		NIST Webbook
rinpol	2652.00		NIST Webbook
tb	886.12	K	Joback Method
tc	1091.62	K	Joback Method
tf	490.96	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.25	J/mol×K	886.12	Joback Method
cpg	1014.95	J/mol×K	920.37	Joback Method
cpg	1030.37	J/mol×K	954.62	Joback Method
cpg	1044.54	J/mol×K	988.87	Joback Method
cpg	1057.48	J/mol×K	1023.12	Joback Method
cpg	1069.24	J/mol×K	1057.37	Joback Method
cpg	1079.83	J/mol×K	1091.62	Joback Method
dvisc	0.0006178	Pa×s	490.96	Joback Method

dvisc	0.0002874	Pa×s	556.82	Joback Method
dvisc	0.0001572	Pa×s	622.68	Joback Method
dvisc	0.0000965	Pa×s	688.54	Joback Method
dvisc	0.0000645	Pa×s	754.40	Joback Method
dvisc	0.0000460	Pa×s	820.26	Joback Method
dvisc	0.0000345	Pa×s	886.12	Joback Method

Sources

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=U415996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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