Pimelic acid, 4-methyl-2-pentyl 1-naphthyl ester

Inchi: InChI=1S/C23H30O4/c1-17(2)16-18(3)26-22(24)14-5-4-6-15-23(25)27-21-13-9-11-19-10
InchiKey: SFRGCKFHPPIRLZ-UHFFFAOYSA-N
Formula: C23H30O4
SMILES: CC(C)CC(C)OC(=O)CCCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-120.51	kJ/mol	Joback Method
hf	-602.08	kJ/mol	Joback Method
hfus	44.52	kJ/mol	Joback Method
hvap	88.91	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	5.674		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	2801.00		NIST Webbook
rinpol	2801.00		NIST Webbook
tb	927.98	K	Joback Method
tc	1146.03	K	Joback Method
tf	534.93	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.58	J/mol×K	927.98	Joback Method
cpg	995.85	J/mol×K	964.32	Joback Method
cpg	1009.93	J/mol×K	1000.66	Joback Method
cpg	1022.88	J/mol×K	1037.01	Joback Method
cpg	1034.76	J/mol×K	1073.35	Joback Method
cpg	1045.63	J/mol×K	1109.69	Joback Method
cpg	1055.56	J/mol×K	1146.03	Joback Method
dvisc	0.0006384	Pa×s	534.93	Joback Method

dvisc	0.0003481	Pa×s	600.44	Joback Method
dvisc	0.0002139	Pa×s	665.95	Joback Method
dvisc	0.0001434	Pa×s	731.46	Joback Method
dvisc	0.0001027	Pa×s	796.96	Joback Method
dvisc	0.0000773	Pa×s	862.47	Joback Method
dvisc	0.0000606	Pa×s	927.98	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=U416720&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