

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

Inchi:	InChI=1S/C23H30O4/c1-17(2)15-18(3)26-22(24)11-5-4-6-12-23(25)27-21-14-13-19-9-7-8
InchiKey:	DBAQFDHUHRAIBF-UHFFFAOYSA-N
Formula:	C23H30O4
SMILES:	CC(C)CC(C)OC(=O)CCCCC(=O)Oc1ccc2ccccc2c1
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	2842.00		NIST Webbook
rinpol	2842.00		NIST Webbook
tb	927.98	K	Joback Method
tc	1146.03	K	Joback Method
tf	534.93	K	Joback Method
vc	1.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003481	Paxs	600.44	Joback Method
dvisc	0.0002139	Paxs	665.95	Joback Method
dvisc	0.0001434	Paxs	731.46	Joback Method
dvisc	0.0001027	Paxs	796.96	Joback Method
dvisc	0.0000773	Paxs	862.47	Joback Method
dvisc	0.0000606	Paxs	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=U416710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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

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