

Pimelic acid, 1-naphthyl nonyl ester

Inchi:

Wmgurydarlosew-UHFFFAOYSA-N

InchiKey:

WMGURYDARLOSEW-UHFFFAOYSA-N

Formula:

C26H36O4

SMILES:

CCCCCCCCCOC(=O)CCCCC(=O)Oc1cccc2ccccc12

Mol. weight [g/mol]:

412.56

Physical Properties

Property code	Value	Unit	Source
gf	-90.37	kJ/mol	Joback Method
hf	-653.44	kJ/mol	Joback Method
hfus	59.34	kJ/mol	Joback Method
hvap	96.36	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	6.989		Crippen Method
mcvol	348.860	ml/mol	McGowan Method
pc	1067.27	kPa	Joback Method
rinpol	3238.00		NIST Webbook
rinpol	3238.00		NIST Webbook
tb	997.50	K	Joback Method
tc	1221.46	K	Joback Method
tf	598.74	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1162.28	J/mol×K	997.50	Joback Method
cpg	1230.19	J/mol×K	1184.14	Joback Method
cpg	1218.80	J/mol×K	1146.81	Joback Method
cpg	1206.39	J/mol×K	1109.48	Joback Method
cpg	1192.88	J/mol×K	1072.15	Joback Method
cpg	1178.20	J/mol×K	1034.83	Joback Method
cpg	1240.65	J/mol×K	1221.46	Joback Method
dvisc	0.0000478	Pa×s	997.50	Joback Method

dvisc	0.0000601	Pa×s	931.04	Joback Method
dvisc	0.0000781	Pa×s	864.58	Joback Method
dvisc	0.0001061	Pa×s	798.12	Joback Method
dvisc	0.0001523	Pa×s	731.66	Joback Method
dvisc	0.0002351	Pa×s	665.20	Joback Method
dvisc	0.0003997	Pa×s	598.74	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=U416725&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

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