

Pimelic acid, 1-naphthyl pentyl ester

Inchi:	InChI=1S/C22H28O4/c1-2-3-9-17-25-21(23)15-5-4-6-16-22(24)26-20-14-10-12-18-11-7-8
InchiKey:	OIWXDIAIGQNZOH-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	356.46

Physical Properties

Property code	Value	Unit	Source
gf	-124.05	kJ/mol	Joback Method
hf	-570.88	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	87.46	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.429		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpola	2843.00		NIST Webbook
tb	905.98	K	Joback Method
tc	1119.89	K	Joback Method
tf	553.66	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.00	J/molxK	905.98	Joback Method
cpg	984.14	J/molxK	1084.24	Joback Method
cpg	973.31	J/molxK	1048.59	Joback Method
cpg	961.53	J/molxK	1012.93	Joback Method
cpg	948.76	J/molxK	977.28	Joback Method
cpg	934.94	J/molxK	941.63	Joback Method
cpg	994.08	J/molxK	1119.89	Joback Method
dvisc	0.0000834	Paxs	905.98	Joback Method
dvisc	0.0001034	Paxs	847.26	Joback Method

dvisc	0.0001322	Paxs	788.54	Joback Method
dvisc	0.0001760	Paxs	729.82	Joback Method
dvisc	0.0002463	Paxs	671.10	Joback Method
dvisc	0.0003677	Paxs	612.38	Joback Method
dvisc	0.0005974	Paxs	553.66	Joback Method

Sources

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=U416721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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