Pimelic acid, heptyl 1-naphthyl ester

Inchi: InChI=1S/C24H32O4/c1-2-3-4-5-11-19-27-23(25)17-7-6-8-18-24(26)28-22-16-12-14-20-1
InchiKey: IBQZDAVXKMXFGS-UHFFFAOYSA-N
Formula: C24H32O4
SMILES: CCCCCCCOC(=O)CCCCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]: 384.51

Physical Properties

Property code	Value	Unit	Source
gf	-107.21	kJ/mol	Joback Method
hf	-612.16	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	91.91	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.209		Crippen Method
mcvol	320.680	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		NIST Webbook
tb	951.74	K	Joback Method
tc	1168.86	K	Joback Method
tf	576.20	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.95	J/mol×K	951.74	Joback Method
cpg	1055.33	J/mol×K	987.93	Joback Method
cpg	1069.55	J/mol×K	1024.11	Joback Method
cpg	1082.66	J/mol×K	1060.30	Joback Method
cpg	1094.73	J/mol×K	1096.49	Joback Method
cpg	1105.83	J/mol×K	1132.67	Joback Method
cpg	1116.02	J/mol×K	1168.86	Joback Method
dvisc	0.0004923	Pa×s	576.20	Joback Method

dvisc	0.0002960	Pa×s	638.79	Joback Method
dvisc	0.0001949	Pa×s	701.38	Joback Method
dvisc	0.0001374	Pa×s	763.97	Joback Method
dvisc	0.0001022	Pa×s	826.56	Joback Method
dvisc	0.0000792	Pa×s	889.15	Joback Method
dvisc	0.0000635	Pa×s	951.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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