Pimelic acid, 2-naphthyl pentyl ester

Inchi: InChI=1S/C22H28O4/c1-2-3-9-16-25-21(23)12-5-4-6-13-22(24)26-20-15-14-18-10-7-8-11
InchiKey: KPHDHDFOGQBVAH-UHFFFAOYSA-N
Formula: C22H28O4
SMILES: CCCCCOC(=O)CCCCCC(=O)Oc1ccc2ccccc2c1
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
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	905.98	K	Joback Method
tc	1119.89	K	Joback Method
tf	553.66	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.00	J/mol×K	905.98	Joback Method
cpg	984.14	J/mol×K	1084.24	Joback Method
cpg	973.31	J/mol×K	1048.59	Joback Method
cpg	961.53	J/mol×K	1012.93	Joback Method
cpg	948.76	J/mol×K	977.28	Joback Method
cpg	934.94	J/mol×K	941.63	Joback Method
cpg	994.08	J/mol×K	1119.89	Joback Method
dvisc	0.0000834	Pa×s	905.98	Joback Method

dvisc	0.0001034	Pa×s	847.26	Joback Method
dvisc	0.0001322	Pa×s	788.54	Joback Method
dvisc	0.0001760	Pa×s	729.82	Joback Method
dvisc	0.0002463	Pa×s	671.10	Joback Method
dvisc	0.0003677	Pa×s	612.38	Joback Method
dvisc	0.0005974	Pa×s	553.66	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=U416711&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