Pimelic acid, hexyl 2-naphthyl ester

Inchi: InChI=1S/C23H30O4/c1-2-3-4-10-17-26-22(24)13-6-5-7-14-23(25)27-21-16-15-19-11-8-9
InchiKey: NDEADIRDUBEQSX-UHFFFAOYSA-N
Formula: C23H30O4
SMILES: CCCCCCOC(=O)CCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 370.48

Physical Properties

Property code	Value	Unit	Source
gf	-115.63	kJ/mol	Joback Method
hf	-591.52	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.819		Crippen Method
mcvol	306.590	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	928.86	K	Joback Method
tc	1143.95	K	Joback Method
tf	564.93	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.65	J/mol×K	928.86	Joback Method
cpg	1044.64	J/mol×K	1108.10	Joback Method
cpg	1033.68	J/mol×K	1072.25	Joback Method
cpg	1021.76	J/mol×K	1036.41	Joback Method
cpg	1008.82	J/mol×K	1000.56	Joback Method
cpg	994.80	J/mol×K	964.71	Joback Method
cpg	1054.71	J/mol×K	1143.95	Joback Method
dvisc	0.0000729	Pa×s	928.86	Joback Method

dvisc	0.0000906	Pa×s	868.20	Joback Method
dvisc	0.0001164	Pa×s	807.55	Joback Method
dvisc	0.0001558	Pa×s	746.89	Joback Method
dvisc	0.0002195	Pa×s	686.24	Joback Method
dvisc	0.0003305	Pa×s	625.59	Joback Method
dvisc	0.0005434	Pa×s	564.93	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=U416712&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