

Pimelic acid, hexyl 1-naphthyl ester

Inchi:	InChI=1S/C23H30O4/c1-2-3-4-10-18-26-22(24)16-6-5-7-17-23(25)27-21-15-11-13-19-12
InchiKey:	RYP AQZLGPXCCPR-UHFFFAOYSA-N
Formula:	C23H30O4
SMILES:	CCCCCOC(=O)CCCCC(=O)Oc1cccc2ccccc12
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
mvol	306.590	ml/mol	McGowan Method
pc	1300.47	kPa	Joback Method
rmpol	2942.00		NIST Webbook
rmpol	2942.00		NIST Webbook
tb	928.86	K	Joback Method
tc	1143.95	K	Joback Method
tf	564.93	K	Joback Method
vc	1.185	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000906	Paxs	868.20	Joback Method
dvisc	0.0001164	Paxs	807.55	Joback Method
dvisc	0.0001558	Paxs	746.89	Joback Method
dvisc	0.0002195	Paxs	686.24	Joback Method
dvisc	0.0003305	Paxs	625.59	Joback Method
dvisc	0.0005434	Paxs	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=U416722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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