

Pimelic acid, heptyl 2-naphthyl ester

Inchi:	InChI=1S/C24H32O4/c1-2-3-4-5-11-18-27-23(25)14-7-6-8-15-24(26)28-22-17-16-20-12-9
InchiKey:	QVLUQCSUIPMPGV-UHFFFAOYSA-N
Formula:	C24H32O4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1ccc2ccccc2c1
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
mvol	320.680	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	3085.00		NIST Webbook
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tb	951.74	K	Joback Method
tc	1168.86	K	Joback Method
tf	576.20	K	Joback Method
vc	1.242	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.95	J/molxK	951.74	Joback Method
cpg	1105.83	J/molxK	1132.67	Joback Method
cpg	1094.73	J/molxK	1096.49	Joback Method
cpg	1082.66	J/molxK	1060.30	Joback Method
cpg	1069.55	J/molxK	1024.11	Joback Method
cpg	1055.33	J/molxK	987.93	Joback Method
cpg	1116.02	J/molxK	1168.86	Joback Method
dvisc	0.0000635	Paxs	951.74	Joback Method

dvisc	0.0000792	Paxs	889.15	Joback Method
dvisc	0.0001022	Paxs	826.56	Joback Method
dvisc	0.0001374	Paxs	763.97	Joback Method
dvisc	0.0001949	Paxs	701.38	Joback Method
dvisc	0.0002960	Paxs	638.79	Joback Method
dvisc	0.0004923	Paxs	576.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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