

Pimelic acid, hexyl undecyl ester

Inchi:	InChI=1S/C24H46O4/c1-3-5-7-9-10-11-12-13-18-22-28-24(26)20-16-14-15-19-23(25)27-
InchiKey:	ZAHPIVPZWKNRJE-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-316.64	kJ/mol	Joback Method
hf	-1028.29	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	87.33	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.134		Crippen Method
mvol	363.900	ml/mol	McGowan Method
pc	849.99	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	901.10	K	Joback Method
tc	1104.70	K	Joback Method
tf	504.56	K	Joback Method
vc	1.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.58	J/molxK	901.10	Joback Method
cpg	1237.78	J/molxK	935.03	Joback Method
cpg	1256.57	J/molxK	968.97	Joback Method
cpg	1273.99	J/molxK	1002.90	Joback Method
cpg	1290.07	J/molxK	1036.83	Joback Method
cpg	1304.84	J/molxK	1070.77	Joback Method
cpg	1318.35	J/molxK	1104.70	Joback Method
dvisc	0.0005261	Paxs	504.56	Joback Method

dvisc	0.0002463	Paxs	570.65	Joback Method
dvisc	0.0001350	Paxs	636.74	Joback Method
dvisc	0.0000828	Paxs	702.83	Joback Method
dvisc	0.0000553	Paxs	768.92	Joback Method
dvisc	0.0000393	Paxs	835.01	Joback Method
dvisc	0.0000294	Paxs	901.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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