Pimelic acid, dodecyl pentyl ester

Inchi: InChI=1S/C24H46O4/c1-3-5-7-8-9-10-11-12-13-18-22-28-24(26)20-16-14-15-19-23(25)2
InchiKey: TVPBZNRDTSTFCG-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=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
mcvol	363.900	ml/mol	McGowan Method
pc	849.99	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	901.10	K	Joback Method
tc	1104.70	K	Joback Method
tf	504.56	K	Joback Method
vc	1.427	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002463	Pa×s	570.65	Joback Method
dvisc	0.0001350	Pa×s	636.74	Joback Method
dvisc	0.0000828	Pa×s	702.83	Joback Method
dvisc	0.0000553	Pa×s	768.92	Joback Method
dvisc	0.0000393	Pa×s	835.01	Joback Method
dvisc	0.0000294	Pa×s	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=U393817&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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