Pimelic acid, hexadecyl propyl ester

Inchi: InChI=1S/C26H50O4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-20-24-30-26(28)22-19-17-18
InchiKey: VWZVHDFXVUQDSW-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-299.80	kJ/mol	Joback Method
hf	-1069.57	kJ/mol	Joback Method
hfus	68.67	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.915		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	762.26	kPa	Joback Method
rinpol	2964.00		NIST Webbook
rinpol	2964.00		NIST Webbook
tb	946.86	K	Joback Method
tc	1166.44	K	Joback Method
tf	527.10	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.23	J/mol×K	946.86	Joback Method
cpg	1366.62	J/mol×K	983.46	Joback Method
cpg	1386.33	J/mol×K	1020.05	Joback Method
cpg	1404.40	J/mol×K	1056.65	Joback Method
cpg	1420.89	J/mol×K	1093.25	Joback Method
cpg	1435.85	J/mol×K	1129.84	Joback Method
cpg	1449.33	J/mol×K	1166.44	Joback Method
dvisc	0.0004085	Pa×s	527.10	Joback Method

dvisc	0.0001878	Pa×s	597.06	Joback Method
dvisc	0.0001016	Pa×s	667.02	Joback Method
dvisc	0.0000618	Pa×s	736.98	Joback Method
dvisc	0.0000410	Pa×s	806.94	Joback Method
dvisc	0.0000290	Pa×s	876.90	Joback Method
dvisc	0.0000216	Pa×s	946.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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