

Pimelic acid, octyl undecyl ester

Inchi:

InChI=1S/C26H50O4/c1-3-5-7-9-11-12-13-15-20-24-30-26(28)22-18-16-17-21-25(27)29-

InchiKey:

UMNIIUWNYSQALM-UHFFFAOYSA-N

Formula:

C26H50O4

SMILES:

CCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC

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	2958.00		NIST Webbook
rinpol	2958.00		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/molxK	946.86	Joback Method
cpg	1435.85	J/molxK	1129.84	Joback Method
cpg	1420.89	J/molxK	1093.25	Joback Method
cpg	1404.40	J/molxK	1056.65	Joback Method
cpg	1386.33	J/molxK	1020.05	Joback Method
cpg	1366.62	J/molxK	983.46	Joback Method
cpg	1449.33	J/molxK	1166.44	Joback Method
dvisc	0.0000216	Paxs	946.86	Joback Method

dvisc	0.0000290	Paxs	876.90	Joback Method
dvisc	0.0000410	Paxs	806.94	Joback Method
dvisc	0.0000618	Paxs	736.98	Joback Method
dvisc	0.0001016	Paxs	667.02	Joback Method
dvisc	0.0001878	Paxs	597.06	Joback Method
dvisc	0.0004085	Paxs	527.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=U393876&Units=SI

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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