

Pimelic acid, undecyl pentyl ester

Inchi:	InChI=1S/C23H44O4/c1-3-5-7-8-9-10-11-12-17-21-27-23(25)19-15-13-14-18-22(24)26-2
InchiKey:	LUEWRULWXXUFEU-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-325.06	kJ/mol	Joback Method
hf	-1007.65	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	85.10	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.744		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	899.64	kPa	Joback Method
rinpol	2665.00		NIST Webbook
rinpol	2665.00		NIST Webbook
tb	878.22	K	Joback Method
tc	1075.46	K	Joback Method
tf	493.29	K	Joback Method
vc	1.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.52	J/molxK	878.22	Joback Method
cpg	1174.19	J/molxK	911.09	Joback Method
cpg	1192.56	J/molxK	943.97	Joback Method
cpg	1209.66	J/molxK	976.84	Joback Method
cpg	1225.52	J/molxK	1009.71	Joback Method
cpg	1240.17	J/molxK	1042.59	Joback Method
cpg	1253.64	J/molxK	1075.46	Joback Method
dvisc	0.0005944	Paxs	493.29	Joback Method

dvisc	0.0002809	Paxs	557.44	Joback Method
dvisc	0.0001550	Paxs	621.60	Joback Method
dvisc	0.0000955	Paxs	685.75	Joback Method
dvisc	0.0000640	Paxs	749.91	Joback Method
dvisc	0.0000457	Paxs	814.07	Joback Method
dvisc	0.0000342	Paxs	878.22	Joback Method

Sources

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=U393816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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