

Pimelic acid, 4-methoxybenzyl undecyl ester

Inchi:	InChI=1S/C26H42O5/c1-3-4-5-6-7-8-9-10-14-21-30-25(27)15-12-11-13-16-26(28)31-22-2
InchiKey:	DZZCXZOOABDCHC-UHFFFAOYSA-N
Formula:	C26H42O5
SMILES:	CCCCCCCCCOC(=O)CCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]:	434.61

Physical Properties

Property code	Value	Unit	Source
gf	-302.02	kJ/mol	Joback Method
hf	-976.73	kJ/mol	Joback Method
hfus	63.51	kJ/mol	Joback Method
hvap	97.13	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.763		Crippen Method
mcvol	374.190	ml/mol	McGowan Method
pc	905.61	kPa	Joback Method
rinpol	1615.00		NIST Webbook
rinpol	1615.00		NIST Webbook
tb	1000.94	K	Joback Method
tc	1227.37	K	Joback Method
tf	588.27	K	Joback Method
vc	1.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1273.11	J/molxK	1000.94	Joback Method
cpg	1289.90	J/molxK	1038.68	Joback Method
cpg	1304.93	J/molxK	1076.42	Joback Method
cpg	1318.22	J/molxK	1114.15	Joback Method
cpg	1329.82	J/molxK	1151.89	Joback Method
cpg	1339.75	J/molxK	1189.63	Joback Method
cpg	1348.07	J/molxK	1227.37	Joback Method
dvisc	0.0002091	Paxs	588.27	Joback Method

dvisc	0.0001102	Paxs	657.05	Joback Method
dvisc	0.0000656	Paxs	725.83	Joback Method
dvisc	0.0000427	Paxs	794.61	Joback Method
dvisc	0.0000298	Paxs	863.38	Joback Method
dvisc	0.0000219	Paxs	932.16	Joback Method
dvisc	0.0000168	Paxs	1000.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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