Pimelic acid, 4-methoxybenzyl nonyl ester

Inchi: InChI=1S/C24H38O5/c1-3-4-5-6-7-8-12-19-28-23(25)13-10-9-11-14-24(26)29-20-21-15-1

InchiKey: ZSVPGWVPZYNLFE-UHFFFAOYSA-N

Formula: C24H38O5

SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)OCc1ccc(OC)cc1

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-318.86	kJ/mol	Joback Method
hf	-935.45	kJ/mol	Joback Method
hfus	58.33	kJ/mol	Joback Method
hvap	92.68	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.983		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook
tb	955.18	K	Joback Method
tc	1169.41	K	Joback Method
tf	565.73	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.17	J/mol×K	955.18	Joback Method
cpg	1216.01	J/mol×K	1133.71	Joback Method
cpg	1205.60	J/mol×K	1098.00	Joback Method
cpg	1193.74	J/mol×K	1062.30	Joback Method
cpg	1180.40	J/mol×K	1026.59	Joback Method
cpg	1165.55	J/mol×K	990.89	Joback Method
cpg	1224.99	J/mol×K	1169.41	Joback Method
dvisc	0.0000228	Pa×s	955.18	Joback Method

dvisc	0.0000296	Pa×s	890.27	Joback Method
dvisc	0.0000400	Pa×s	825.36	Joback Method
dvisc	0.0000569	Pa×s	760.45	Joback Method
dvisc	0.0000864	Pa×s	695.55	Joback Method
dvisc	0.0001432	Pa×s	630.64	Joback Method
dvisc	0.0002663	Pa×s	565.73	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=U416544&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