Pimelic acid, hexyl 1-methoxydec-4-yl ester

Inchi: InChI=1S/C24H46O5/c1-4-6-8-11-16-22(17-15-20-27-3)29-24(26)19-13-10-12-18-23(25)28-21-14-9-7-5-2/h22H,4-21H2,1-3H3

InchiKey: AGBXPIZAMVRIQX-UHFFFAOYSA-N

Formula: C24H46O5

SMILES: CCCCCCOC(=O)CCCCCC(=O)OC(CCCCCC)CCCOC

Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-424.08	kJ/mol	Joback Method
hf	-1165.79	kJ/mol	Joback Method
hfus	61.16	kJ/mol	Joback Method
hvap	89.35	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.369		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	845.54	kPa	Joback Method
rinpol	2689.00		NIST Webbook
rinpol	2689.00		NIST Webbook
tb	923.08	K	Joback Method
tc	1132.65	K	Joback Method
tf	511.79	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.13	J/mol×K	923.08	Joback Method
cpg	1333.37	J/mol×K	1097.72	Joback Method
cpg	1319.81	J/mol×K	1062.79	Joback Method
cpg	1304.72	J/mol×K	1027.86	Joback Method
cpg	1288.10	J/mol×K	992.94	Joback Method
cpg	1269.91	J/mol×K	958.01	Joback Method
cpg	1345.43	J/mol×K	1132.65	Joback Method
dvisc	0.0000198	Pa×s	923.08	Joback Method

dvisc	0.0000268	Pa×s	854.53	Joback Method
dvisc	0.0000382	Pa×s	785.98	Joback Method
dvisc	0.0000582	Pa×s	717.43	Joback Method
dvisc	0.0000969	Pa×s	648.89	Joback Method
dvisc	0.0001821	Pa×s	580.34	Joback Method
dvisc	0.0004053	Pa×s	511.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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