Pimelic acid, dodecyl 5-methoxy-3-methylpent-2-yl ester

Inchi: InChI=1S/C26H50O5/c1-5-6-7-8-9-10-11-12-13-17-21-30-25(27)18-15-14-16-19-26(28)3
InchiKey: QIEALWZDKSJBAV-UHFFFAOYSA-N
Formula: C26H50O5
SMILES: CCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]: 442.67

Physical Properties

Property code	Value	Unit	Source
gf	-409.68	kJ/mol	Joback Method
hf	-1212.35	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	93.42	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.005		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	761.84	kPa	Joback Method
rinpol	2947.00		NIST Webbook
rinpol	2947.00		NIST Webbook
tb	968.40	K	Joback Method
tc	1193.44	K	Joback Method
tf	519.33	K	Joback Method
vc	1.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.84	J/mol×K	968.40	Joback Method
cpg	1461.96	J/mol×K	1155.94	Joback Method
cpg	1448.82	J/mol×K	1118.43	Joback Method
cpg	1433.87	J/mol×K	1080.92	Joback Method
cpg	1417.09	J/mol×K	1043.41	Joback Method
cpg	1398.42	J/mol×K	1005.91	Joback Method
cpg	1473.33	J/mol×K	1193.44	Joback Method
dvisc	0.0000132	Pa×s	968.40	Joback Method

dvisc	0.0000181	Pa×s	893.56	Joback Method
dvisc	0.0000264	Pa×s	818.71	Joback Method
dvisc	0.0000416	Pa×s	743.87	Joback Method
dvisc	0.0000725	Pa×s	669.02	Joback Method
dvisc	0.0001454	Pa×s	594.17	Joback Method
dvisc	0.0003561	Pa×s	519.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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