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

Inchi: InChI=1S/C23H44O5/c1-5-6-7-8-9-10-14-18-27-22(24)15-12-11-13-16-23(25)28-21(3)20

InchiKey: PHKCIBBKAKQSBD-UHFFFAOYSA-N

Formula: C23H44O5

SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CCOC

Mol. weight [g/mol]: 400.59

Physical Properties

Property code	Value	Unit	Source
gf	-434.94	kJ/mol	Joback Method
hf	-1150.43	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.835		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	899.76	K	Joback Method
tc	1101.93	K	Joback Method
tf	485.52	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.52	J/mol×K	899.76	Joback Method
cpg	1206.77	J/mol×K	933.46	Joback Method
cpg	1224.57	J/mol×K	967.15	Joback Method
cpg	1240.93	J/mol×K	1000.85	Joback Method
cpg	1255.86	J/mol×K	1034.54	Joback Method
cpg	1269.40	J/mol×K	1068.24	Joback Method
cpg	1281.54	J/mol×K	1101.93	Joback Method
dvisc	0.0005368	Pa×s	485.52	Joback Method

dvisc	0.0002239	Pa×s	554.56	Joback Method
dvisc	0.0001133	Pa×s	623.60	Joback Method
dvisc	0.0000657	Pa×s	692.64	Joback Method
dvisc	0.0000421	Pa×s	761.68	Joback Method
dvisc	0.0000290	Pa×s	830.72	Joback Method
dvisc	0.0000212	Pa×s	899.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406722&Units=SI

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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