Pimelic acid, decyl 3-(2-methoxyethyl)nonyl ester

Inchi: InChI=1S/C29H56O5/c1-4-6-8-10-11-12-13-18-24-33-28(30)20-16-14-17-21-29(31)34-26

InchiKey: YUZIESVXHMGNFT-UHFFFAOYSA-N

Formula: C29H56O5

SMILES: CCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(CCCCCC)CCOC

Mol. weight [g/mol]: 484.75

Physical Properties

Property code	Value	Unit	Source
gf	-381.98	kJ/mol	Joback Method
hf	-1268.99	kJ/mol	Joback Method
hfus	74.10	kJ/mol	Joback Method
hvap	100.48	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.177		Crippen Method
mcvol	440.220	ml/mol	McGowan Method
pc	651.10	kPa	Joback Method
rinpol	3232.00		NIST Webbook
rinpol	3232.00		NIST Webbook
tb	1037.48	K	Joback Method
tc	1300.17	K	Joback Method
tf	568.14	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1570.96	J/mol×K	1037.48	Joback Method
cpg	1593.43	J/mol×K	1081.26	Joback Method
cpg	1613.23	J/mol×K	1125.04	Joback Method
cpg	1630.43	J/mol×K	1168.83	Joback Method
cpg	1645.12	J/mol×K	1212.61	Joback Method
cpg	1657.35	J/mol×K	1256.39	Joback Method
cpg	1667.22	J/mol×K	1300.17	Joback Method
dvisc	0.0002050	Pa×s	568.14	Joback Method

dvisc	0.0000886	Pa×s	646.36	Joback Method
dvisc	0.0000459	Pa×s	724.59	Joback Method
dvisc	0.0000270	Pa×s	802.81	Joback Method
dvisc	0.0000175	Pa×s	881.03	Joback Method
dvisc	0.0000121	Pa×s	959.26	Joback Method
dvisc	0.0000089	Pa×s	1037.48	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=U406764&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