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

Inchi: InChI=1S/C28H54O5/c1-4-6-8-10-11-12-17-23-32-27(29)19-15-13-16-20-28(30)33-25-22
InchiKey: KWGMYWOSLHWLJO-UHFFFAOYSA-N
Formula: C28H54O5
SMILES: CCCCCCCCCOC(=O)CCCCCC(=O)OCCC(CCCCCC)CCOC
Mol. weight [g/mol]: 470.73

Physical Properties

Property code	Value	Unit	Source
gf	-390.40	kJ/mol	Joback Method
hf	-1248.35	kJ/mol	Joback Method
hfus	71.52	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.787		Crippen Method
mcvol	426.130	ml/mol	McGowan Method
pc	684.21	kPa	Joback Method
rinpol	3135.00		NIST Webbook
rinpol	3135.00		NIST Webbook
tb	1014.60	K	Joback Method
tc	1263.85	K	Joback Method
tf	556.87	K	Joback Method
vc	1.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.22	J/mol×K	1014.60	Joback Method
cpg	1528.11	J/mol×K	1056.14	Joback Method
cpg	1547.60	J/mol×K	1097.68	Joback Method
cpg	1564.77	J/mol×K	1139.22	Joback Method
cpg	1579.67	J/mol×K	1180.76	Joback Method
cpg	1592.37	J/mol×K	1222.30	Joback Method
cpg	1602.91	J/mol×K	1263.85	Joback Method
dvisc	0.0002359	Pa×s	556.87	Joback Method

dvisc	0.0001027	Pa×s	633.16	Joback Method
dvisc	0.0000535	Pa×s	709.45	Joback Method
dvisc	0.0000316	Pa×s	785.73	Joback Method
dvisc	0.0000205	Pa×s	862.02	Joback Method
dvisc	0.0000143	Pa×s	938.31	Joback Method
dvisc	0.0000105	Pa×s	1014.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406763&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

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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