Pimelic acid, 3-(2-methoxyethyl)heptyl octyl ester

Inchi: InChI=1S/C25H48O5/c1-4-6-8-9-10-14-20-29-24(26)16-12-11-13-17-25(27)30-22-19-23(

InchiKey: UNWBODITQRQZBH-UHFFFAOYSA-N

Formula: C25H48O5

SMILES: CCCCCCCCOC(=O)CCCCCC(=O)OCCC(CCCC)CCOC

Mol. weight [g/mol]: 428.65

Physical Properties

Property code	Value	Unit	Source
gf	-415.66	kJ/mol	Joback Method
hf	-1186.43	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.617		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	2857.00		NIST Webbook
rinpol	2857.00		NIST Webbook
tb	945.96	K	Joback Method
tc	1163.54	K	Joback Method
tf	523.06	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.62	J/mol×K	945.96	Joback Method
cpg	1397.77	J/mol×K	1127.28	Joback Method
cpg	1384.32	J/mol×K	1091.02	Joback Method
cpg	1369.21	J/mol×K	1054.75	Joback Method
cpg	1352.40	J/mol×K	1018.49	Joback Method
cpg	1333.88	J/mol×K	982.22	Joback Method
cpg	1409.59	J/mol×K	1163.54	Joback Method
dvisc	0.0000169	Pa×s	945.96	Joback Method

dvisc	0.0000229	Pa×s	875.48	Joback Method
dvisc	0.0000327	Pa×s	804.99	Joback Method
dvisc	0.0000501	Pa×s	734.51	Joback Method
dvisc	0.0000837	Pa×s	664.03	Joback Method
dvisc	0.0001583	Pa×s	593.54	Joback Method
dvisc	0.0003553	Pa×s	523.06	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=U406787&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