Pimelic acid, 2-(2-methoxyethyl)heptyl 4-methyl-2-pentyl ester

Inchi: InChI=1S/C23H44O5/c1-6-7-9-12-21(15-16-26-5)18-27-22(24)13-10-8-11-14-23(25)28-2

InchiKey: BEKBNVBFIPJUAC-UHFFFAOYSA-N

Formula: C23H44O5

SMILES: CCCCCC(CCOC)COC(=O)CCCCCC(=O)OC(C)CC(C)C

Mol. weight [g/mol]: 400.59

Physical Properties

Property code	Value	Unit	Source
gf	-437.38	kJ/mol	Joback Method
hf	-1155.71	kJ/mol	Joback Method
hfus	51.52	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.691		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	903.43	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	899.32	K	Joback Method
tc	1101.14	K	Joback Method
tf	470.52	K	Joback Method
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.95	J/mol×K	899.32	Joback Method
cpg	1207.15	J/mol×K	932.96	Joback Method
cpg	1224.89	J/mol×K	966.59	Joback Method
cpg	1241.18	J/mol×K	1000.23	Joback Method
cpg	1256.04	J/mol×K	1033.86	Joback Method
cpg	1269.50	J/mol×K	1067.50	Joback Method
cpg	1281.56	J/mol×K	1101.14	Joback Method
dvisc	0.0006365	Pa×s	470.52	Joback Method

dvisc	0.0002422	Pa×s	541.99	Joback Method
dvisc	0.0001154	Pa×s	613.45	Joback Method
dvisc	0.0000642	Pa×s	684.92	Joback Method
dvisc	0.0000399	Pa×s	756.39	Joback Method
dvisc	0.0000269	Pa×s	827.85	Joback Method
dvisc	0.0000193	Pa×s	899.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406733&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