Pimelic acid, di(2-(2-methoxyethyl)hexyl) ester

Inchi: InChI=1S/C25H48O6/c1-5-7-12-22(16-18-28-3)20-30-24(26)14-10-9-11-15-25(27)31-21-
InchiKey: WVBXPEDPLDLCJD-UHFFFAOYSA-N
Formula: C25H48O6
SMILES: CCCCC(CCOC)COC(=O)CCCCCC(=O)OCC(CCCC)CCOC
Mol. weight [g/mol]: 444.64

Physical Properties

Property code	Value	Unit	Source
gf	-523.10	kJ/mol	Joback Method
hf	-1323.93	kJ/mol	Joback Method
hfus	61.41	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	5.709		Crippen Method
mcvol	389.730	ml/mol	McGowan Method
pc	796.18	kPa	Joback Method
rinpol	2861.00		NIST Webbook
rinpol	2861.00		NIST Webbook
tb	967.94	K	Joback Method
tc	1192.43	K	Joback Method
tf	530.29	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.33	J/mol×K	967.94	Joback Method
cpg	1423.22	J/mol×K	1155.02	Joback Method
cpg	1411.59	J/mol×K	1117.60	Joback Method
cpg	1398.01	J/mol×K	1080.19	Joback Method
cpg	1382.45	J/mol×K	1042.77	Joback Method
cpg	1364.89	J/mol×K	1005.36	Joback Method
cpg	1432.90	J/mol×K	1192.43	Joback Method
dvisc	0.0000113	Pa×s	967.94	Joback Method

dvisc	0.0000155	Pa×s	895.00	Joback Method
dvisc	0.0000224	Pa×s	822.06	Joback Method
dvisc	0.0000348	Pa×s	749.12	Joback Method
dvisc	0.0000594	Pa×s	676.17	Joback Method
dvisc	0.0001156	Pa×s	603.23	Joback Method
dvisc	0.0002700	Pa×s	530.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406753&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