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

Inchi: InChI=1S/C26H50O5/c1-4-6-8-9-10-11-15-21-30-25(27)17-13-12-14-18-26(28)31-23-20-

InchiKey: KEGSDYYGZVHWKE-UHFFFAOYSA-N

Formula: C26H50O5

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

Mol. weight [g/mol]: 442.67

Physical Properties

Property code	Value	Unit	Source
gf	-407.24	kJ/mol	Joback Method
hf	-1207.07	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	93.80	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	7.007		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	758.49	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	968.84	K	Joback Method
tc	1195.64	K	Joback Method
tf	534.33	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.50	J/mol×K	968.84	Joback Method
cpg	1462.47	J/mol×K	1157.84	Joback Method
cpg	1449.19	J/mol×K	1120.04	Joback Method
cpg	1434.09	J/mol×K	1082.24	Joback Method
cpg	1417.13	J/mol×K	1044.44	Joback Method
cpg	1398.28	J/mol×K	1006.64	Joback Method
cpg	1473.97	J/mol×K	1195.64	Joback Method
dvisc	0.0000145	Pa×s	968.84	Joback Method

dvisc	0.0000196	Pa×s	896.42	Joback Method
dvisc	0.0000281	Pa×s	824.00	Joback Method
dvisc	0.0000430	Pa×s	751.58	Joback Method
dvisc	0.0000722	Pa×s	679.17	Joback Method
dvisc	0.0001373	Pa×s	606.75	Joback Method
dvisc	0.0003107	Pa×s	534.33	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406788&Units=SI

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