Pimelic acid, pentadecyl 3-methylbutyl ester

Inchi: InChI=1S/C27H52O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-23-30-26(28)20-17-16-18-21
InchiKey: KDOQRTPYHSBKJG-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-293.82	kJ/mol	Joback Method
hf	-1095.49	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.161		Crippen Method
mcvol	406.170	ml/mol	McGowan Method
pc	726.53	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	969.30	K	Joback Method
tc	1196.72	K	Joback Method
tf	523.37	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.04	J/mol×K	969.30	Joback Method
cpg	1431.86	J/mol×K	1007.20	Joback Method
cpg	1451.85	J/mol×K	1045.11	Joback Method
cpg	1470.06	J/mol×K	1083.01	Joback Method
cpg	1486.55	J/mol×K	1120.91	Joback Method
cpg	1501.39	J/mol×K	1158.81	Joback Method
cpg	1514.63	J/mol×K	1196.72	Joback Method
dvisc	0.0004080	Pa×s	523.37	Joback Method

dvisc	0.0001723	Pa×s	597.69	Joback Method
dvisc	0.0000881	Pa×s	672.01	Joback Method
dvisc	0.0000515	Pa×s	746.34	Joback Method
dvisc	0.0000331	Pa×s	820.66	Joback Method
dvisc	0.0000230	Pa×s	894.98	Joback Method
dvisc	0.0000168	Pa×s	969.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393783&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